Lis User Guide Version 1.8.7



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## Changes from Version 1.0

- 1. Addition: Support for double-double (quadruple) precision operations.
- 2. Addition: Support for Fortran compilers.
- 3. Addition: Support for Autotools.
- 4. Changes:
  - (a) Structure of solvers.
  - (b) Arguments of the functions lis\_matrix\_create() and lis\_vector\_create().
  - (c) Notation of command line options.

## Changes from Version 1.1

- 1. Addition: Support for standard eigenvalue problems.
- 2. Addition: Support for 64bit integers.
- 3. Changes:
  - (a) Names of the functions lis\_output\_residual\_history() and lis\_get\_residual\_history() to lis\_solver\_output\_rhistory() and lis\_solver\_get\_rhistory(), respectively.
  - (b) Origin of the Fortran interfaces lis\_vector\_set\_value() and lis\_vector\_get\_value() to 1.
  - (c) Origin of the Fortran interface lis\_vector\_set\_size() to 1.
  - (d) Name of the precision flag -precision to -f.
- 4. Change: Specification of the function lis\_solve\_kernel() to return the residual computed by the function lis\_solve\_execute().
- 5. Changes: Specifications of integer types:
  - (a) Replacement: The type of integer in C programs with LIS\_INT, which is equivalent to int by default. If the preprossor macro \_LONGLONG is defined, it is replaced with long long int.
  - (b) Replacement: The type of integer in Fortran programs with LIS\_INTEGER, which is equivalent to integer by default. If the preprossor macro LONGLONG is defined, it is replaced with integer\*8.
- 6. Change: Names of the matrix storage formats CRS (Compressed Row Storage) and CCS (Compressed Column Storage) to CSR (Compressed Sparse Row) and CSC (Compressed Sparse Column), respectively.
- 7. Change: Names of the functions lis\_get\_solvername(), lis\_get\_preconname(), and lis\_get\_esolvername() to lis\_solver\_get\_solvername(), lis\_solver\_get\_preconname(), and lis\_esolver\_get\_esolvername(), respectively.

## Changes from Version 1.2

- 1. Addition: Support for nmake.
- 2. Change: Name of the file lis\_config\_win32.h to lis\_config\_win.h.
- 3. Change: Name of the matrix storage format JDS (Jagged Diagonal Storage) to JAD (Jagged Diagonal).
- 4. Change: Names of the functions lis\_fscan\_double() and lis\_bswap\_double() to lis\_fscan\_scalar() and lis\_bswap\_scalar(), respectively.

## Changes from Version 1.3

- 1. Addition: Support for long double (quadruple) precision operations.
- 2. Addition: Support for pointer operations in Fortran.
- 3. Change: Name of the members residual of the structs LIS\_SOLVER and LIS\_ESOLVER to rhistory.
- 4. Change: Names of the members iters and iters2 of the structs LIS\_SOLVER and LIS\_ESOLVER to iter and iter2, respectively.
- 5. Change: Names of the functions lis\_solver\_get\_iters(), lis\_solver\_get\_itersex(), lis\_esolver\_get\_iters(), and lis\_esolver\_get\_itersex() to lis\_solver\_get\_iter(), lis\_solver\_get\_iterex(), lis\_esolver\_get\_iter(), and lis\_esolver\_get\_iterex(), respectively.
- 6. Change: Names of the members \*times of the structs LIS\_SOLVER and LIS\_ESOLVER to \*time, respectively.
- 7. Addition: Member intvalue to the struct LIS\_VECTOR.
- 8. Change: Specifications of the functions lis\_output\_vector\*() and lis\_output\_mm\_vec() to allow integer data.
- 9. Change: Names of the functions lis\_matrix\_scaling\*() to lis\_matrix\_scale\*(), respectively.
- 10. Change: Names of the functions lis\_array\_dot2() and lis\_array\_invGauss() to lis\_array\_dot() and lis\_array\_ge(), respectively.

## Changes from Version 1.4

- 1. Addition: Support for array operations.
- 2. Addition: Support for alternative workflow PSD (Preconditioner and Solver Decoupled).
- 3. Change: Specification of the function <code>lis\_array\_qr()</code> to return the number of iterations and error of the QR algorithm.
- 4. Change: Names of the functions lis\_array\_matvec2() and lis\_array\_matmat2() to lis\_array\_matvec\_ns() and lis\_array\_matmat\_ns(), respectively.
- 5. Change: Names of the preprossor macros \_LONGLONG and LONGLONG to \_LONG\_\_LONG and LONG\_\_LONG, respectively.

## Changes from Version 1.5

1. Addition: Support for complex arithmetic.

## Changes from Version 1.6

- 1. Addition: Support for generalized eigenvalue problems.
- 2. Addition: Support for GCC libquadmath.
- 3. Change: Sign of shift for eigensolvers in accordance with custom.
- 4. Change: Sign of shift in lis\_matrix\_shift\_diagonal(), lis\_vector\_shift(), and lis\_array\_shift(), respectively.

## Changes from Version 1.7

- 1. Addition: Support for multiple-step linear equations.
- 2. Names of the flags -ssor\_w and -hybrid\_w to -ssor\_omega and -hybrid\_omega, respectively.

## 1 Introduction

Lis (Library of Iterative Solvers for linear systems, pronounced [lis]) is a parallel software library for solving the linear equations

$$Ax = b$$

and the eigenvalue problems

$$Ax = \lambda Bx$$

with sparse matrices, which arise in the numerical solution of partial differential equations, using iterative methods[1]. The solvers available in Lis are listed in Table 1 and 2, and the preconditioners are listed in Table 3. The supported matrix storage formats are listed in Table 4.

Table 1: Linear Solvers

Table 1. Linear borvers				
CG[2, 3]	CR[2]			
BiCG[4]	BiCR[5]			
CGS[6]	CRS[7]			
BiCGSTAB[8]	BiCRSTAB[7]			
GPBiCG[9]	GPBiCR[7]			
BiCGSafe[10]	BiCRSafe[11]			
BiCGSTAB(1)[12]	TFQMR[13]			
Jacobi[14]	Orthomin(m)[15]			
Gauss-Seidel[16, 17]	GMRES(m)[18]			
SOR[19, 20]	FGMRES(m)[21]			
IDR(s)[22]	MINRES[23]			
COCG[24]	COCR[25]			

Table 2: Eigensolvers

Power[26]
Inverse[27]
Rayleigh Quotient[28]
CG[29]
CR[30]
Subspace[31]
Lanczos[32]
Arnoldi[33]

Table 3: Preconditioners

Table 4: Matrix Storage Formats

	Table 1. Matha Storage Formats		
Jacobi[34]	Compressed Sparse Row	(CSR)	
SSOR[34]	Compressed Sparse Column	(CSC)	
ILU(k)[35, 36]	Modified Compressed Sparse Row	(MSR)	
ILUT[37, 38]	Diagonal	(DIA)	
Crout ILU[38, 39]	Ellpack-Itpack Generalized Diagonal	(ELL)	
I + S[40]	Jagged Diagonal	(JAD)	
SA-AMG[41]	Block Sparse Row	(BSR)	
Hybrid[42]	Block Sparse Column	(BSC)	
SAINV[43]	Variable Block Row	(VBR)	
Additive Schwarz[44, 45]	Coordinate	(COO)	
User defined	Dense	(DNS)	

## 2 Installation

This section describes the instructions for installing and testing Lis.

### 2.1 System Requirements

The installation of Lis requires a C compiler. The Fortran interface requires a Fortran compiler, and the algebraic multigrid preconditioner requires a Fortran 90 compiler. For parallel computing environments, an OpenMP[87] or MPI-1[81] library is used[46, 47]. Both the Harwell-Boeing[73] and Matrix Market[77] formats are supported to import and export user data. Lis has been tested in the environments listed in Table 5 (see also Table 7).

C Compilers OS Intel C/C++ Compiler 7.0, 8.0, 9.1, 10.1, 11.1, 12.1, 14.0, 16.0, 17.0 Linux Windows IBM XL C/C++ V7.0, 9.0 AIX Linux Sun WorkShop 6, Sun ONE Studio 7, Solaris Sun Studio 11, 12 PGI C++ 6.0, 7.1, 10.5, 16.10 Linux gcc 3.3, 4.4, 5.4 Linux Mac OS X Windows Microsoft Visual C++ 2008, 2010, 2012, 2013, 2015, 2017 Windows OS Fortran Compilers (Optional) Intel Fortran Compiler 8.1, 9.1, 10.1, 11.1, 12.1, 14.0, 16.0, 17.0 Linux Windows IBM XL Fortran V9.1, 11.1 AIX Linux Sun WorkShop 6, Sun ONE Studio 7, Solaris Sun Studio 11, 12 PGI Fortran 6.0, 7.1, 10.5, 16.10 Linux g77 3.3 Linux  ${\operatorname{Mac}}$  OS X gfortran 4.4, 5.4

Windows

Table 5: Major Tested Platforms

## 2.2 Installing on UNIX and Compatible Systems

#### 2.2.1 Extracting Archive

Enter the following command to extract the archive, where (\$VERSION) represents the version: > gunzip -c lis-(\$VERSION).tar.gz | tar xvf -

This creates a directory lis-(\$VERSION) together with its subfolders as shown in Figure 1.

#### 2.2.2 Configuring Source Tree

In the directory lis-(\$VERSION), run the following command to configure the source tree:

- default: > ./configure
- specify the installation destination: > ./configure --prefix=<install-dir>

Figure 1: Files contained in lis-(\$VERSION).tar.gz

Table 6 shows the major options that can be specified for the configuration, and Table 7 shows the major computing environments that can be specified by TARGET.

#### 2.2.3 Compiling

In the directory lis-(\$VERSION), run the following command to generate the executable files:

> make

To ensure that the library has been built successfully, enter

> make check

in lis-(\$VERSION). This runs a test script using the executable files created in lis-(\$VERSION)/test, which reads the data of the coefficient matrix and the right-hand side vector from the file test/testmat.mtx and solve the linear equation Ax = b by the BiCG method. The result on the SGI Altix 3700 is shown below. Options --enable-omp and --enable-mpi can be combined.

```
– Default –
matrix size = 100 x 100 (460 nonzero entries)
initial vector x
                     : all components set to 0
precision
                     : double
                     : BiCG
linear solver
preconditioner
                     : none
convergence condition : ||b-Ax||_2 \le 1.0e-12 * ||b-Ax_0||_2
matrix storage format : CSR
linear solver status : normal end
BiCG: number of iterations = 15 (double = 15, quad = 0)
BiCG: elapsed time = 5.178690e-03 sec.
BiCG:
        preconditioner
                        = 1.277685e-03 sec.
BiCG:
        matrix creation = 1.254797e-03 sec.
BiCG: linear solver = 3.901005e-03 sec.
BiCG: relative residual = 6.327297e-15
```

Table 6: Major Configuration Options (see ./configure --help for the complete list)

enable-omp	Build with OpenMP library		
-	2 0		
enable-mpi	Build with MPI library		
enable-fortran	Enable FORTRAN 77 compatible interface		
enable-f90	Enable Fortran 90 compatible interface		
enable-saamg	Enable SA-AMG preconditioner		
enable-quad	Enable double-double (quadruple) precision support		
enable-longdouble	Enable long double (quadruple) precision support		
enable-longlong	Enable 64bit integer support		
enable-complex	Enable complex scalar support		
enable-debug	Enable debugging		
enable-shared	Enable dynamic linking		
enable-gprof	Enable profiling		
prefix= <install-dir></install-dir>	Specify installation destination		
TARGET= <target></target>	Specify computing environment		
CC= <c_compiler></c_compiler>	Specify C compiler		
CFLAGS= <c_flags></c_flags>	Specify options for C compiler		
F77= <f77_compiler></f77_compiler>	Specify FORTRAN 77 compiler		
F77FLAGS= <f77_flags></f77_flags>	Specify options for FORTRAN 77 compiler		
FC= <f90_compiler></f90_compiler>	Specify Fortran 90 compiler		
FCFLAGS= <f90_flags></f90_flags>	Specify options for Fortran 90 compiler		
LDFLAGS=<1d_flags>	Specify link options		

```
---enable-omp —
max number of threads = 32
number of threads = 2
matrix size = 100 x 100 (460 nonzero entries)
initial vector \mathbf{x} \phantom{\mathbf{x}} : all components set to \mathbf{0}
precision
                     : double
linear solver
                     : BiCG
preconditioner
                   : none
convergence condition : ||b-Ax||_2 \le 1.0e-12 * ||b-Ax_0||_2
matrix storage format : CSR
linear solver status : normal end
BiCG: number of iterations = 15 (double = 15, quad = 0)
BiCG: elapsed time = 8.960009e-03 sec. BiCG: preconditioner = 2.297878e-03 sec.
BiCG:
        matrix creation = 2.072096e-03 sec.
BiCG: linear solver = 6.662130e-03 sec.
BiCG: relative residual = 6.221213e-15
```

Table 7: Examples of Targets (see lis-(\$VERSION)/configure.ac for details)

<target></target>	Equivalent options			
cray_xt3_cross	./configure CC=cc FC=ftn CFLAGS="-03 -B -fastsse -tp k8-64"			
	FCFLAGS="-03 -fastsse -tp k8-64 -Mpreprocess" FCLDFLAGS="-Mnomain"			
	ac_cv_sizeof_void_p=8 cross_compiling=yes			
	ax_f77_mangling="lower case, no underscore, extra underscore"			
fujitsu_fx10_cross	./configure CC=fccpx FC=frtpx CFLAGS="-Kfast,ocl,preex"			
	FCFLAGS="-Kfast,ocl,preex -Cpp -fs" FCLDFLAGS="-mlcmain=main"			
	ac_cv_sizeof_void_p=8 cross_compiling=yes			
	ax_f77_mangling="lower case, underscore, no extra underscore"			
hitachi_sr16k	./configure CC=cc FC=f90 CFLAGS="-Os -noparallel"			
	FCFLAGS="-Oss -noparallel" FCLDFLAGS="-1f90s"			
	ac_cv_sizeof_void_p=8			
	ax_f77_mangling="lower case, underscore, no extra underscore"			
ibm_bgl_cross	./configure CC=blrts_xlc FC=blrts_xlf90			
	CFLAGS="-03 -qarch=440d -qtune=440 -qstrict"			
	FCFLAGS="-03 -qarch=440d -qtune=440 -qsuffix=cpp=F90"			
	ac_cv_sizeof_void_p=4 cross_compiling=yes			
	<pre>ax_f77_mangling="lower case, no underscore, no extra underscore"</pre>			
intel_mic_cross	./configure CC=icc F77=ifort FC=ifort			
	MPICC=mpiicc MPIF77=mpiifort MPIFC=mpiifort			
	CFLAGS="-mmic" FFLAGS="-mmic"			
	LDFLAGS="-mmic" FCLDFLAGS="-mmic" cross_compiling=yes			
	host=x86_64-pc-linux-gnu host_alias=x86_64-linux-gnu			
	host_cpu=x86_64 host_os=linux-gnu host_vendor=pc			
	target=k1om-mpss-linux-gnu target_alias=k1om-mpss-linux			
	target_cpu=k1om target_os=linux-gnu target_vendor=mpss			
nec_sx9_cross	./configure CC=sxmpic++ FC=sxmpif90 AR=sxar RANLIB=true			
	<pre>ac_cv_sizeof_void_p=8 ax_vector_machine=yes cross_compiling=yes</pre>			
	ax_f77_mangling="lower case, no underscore, extra underscore"			

```
- --enable-mpi -
number of processes = 2
matrix size = 100 x 100 (460 nonzero entries)
initial vector x
                     : all components set to 0
                     : double
precision
                     : BiCG
linear solver
preconditioner
                    : none
convergence condition : ||b-Ax||_2 \le 1.0e-12 * ||b-Ax_0||_2
matrix storage format : CSR
linear solver status : normal end
BiCG: number of iterations = 15 (double = 15, quad = 0)
BiCG: elapsed time = 2.911400e-03 sec.
                        = 1.560780e-04 \text{ sec.}
BiCG:
       preconditioner
BiCG:
         matrix creation = 1.459997e-04 sec.
BiCG:
        linear solver = 2.755322e-03 sec.
BiCG: relative residual = 6.221213e-15
```

## 2.2.4 Installing

In the directory lis-(\$VERSION), enter

> make install

which copies the files to the destination directory as follows:

lis\_config.h is the header file required to build the library, and lis.h and lisf.h are the header files required by the C and Fortran compilers, respectively. liblis.a is the library. To ensure that the library has been installed successfully, enter

> make installcheck

in lis-(\$VERSION). This runs a test script using the executable files installed in examples/lis. test1, etest5, getest5, test3b, and spmvtest3b in examples/lis are copied in (\$INSTALLDIR)/bin as lsolve, esolve, gesolve, hpcg\_kernel, and hpcg\_spmvtest, respectively. examples/lis/spmvtest\* are also copied in

(\$INSTALLDIR)/bin.

To remove the copied files in (\$INSTALLDIR), enter

> make uninstall

To remove the generated library and executable files in lis-(\$VERSION), enter

> make clean

To remove the configuration files in addition to the other generated files, enter

> make distclean

### 2.3 Installing on Windows Systems

Use an appropriate tool to extract the archive. To use the Microsoft Build Engine, run the following command in the directory lis-(\$VERSION)\win and generate the configuration file Makefile (See configure.bat --help for details):

> configure.bat

The default configuration of Makefile is defined in Makefile.in. To build the library, run the following command in the directory lis-(\$VERSION)\win:

> nmake

To ensure that the library has been built successfully, enter

> nmake check

The following command copies the library to (\$INSTALLDIR)\lib, the executable files to (\$INSTALLDIR)\bin, the header files to (\$INSTALLDIR)\include, and the PDF documents to (\$INSTALLDIR)\doc, respectively:

> nmake install

To remove the copied files in (\$INSTALLDIR), enter

> nmake uninstall

To remove the generated library and executables files in lis-(\$VERSION)\win, enter

> nmake clean

To remove the configuration files in addition to the other generated files, enter

> nmake distclean

To use UNIX compatible environments, follow the instructions in the previous section.

### 2.4 Testing

Test programs are located in lis-(\$VERSION)/test.

#### 2.4.1 test1

Usage: test1 matrix\_filename rhs\_setting solution\_filename rhistory\_filename [options]

This program inputs the data of the coefficient matrix from matrix\_filename and solves the linear equation Ax = b with the solver specified by options. It outputs the solution to solution\_filename in the extended Matrix Market format and the residual history to rhistory\_filename in the PLAIN format (see Appendix). Both the extended Matrix Market format and the Harwell-Boeing format are supported for matrix\_filename. One of the following values can be specified by rhs\_setting:

0 Use the right-hand side vector b included in the data file

1 Use  $b = (1, ..., 1)^T$ 

Use  $b = A \times (1, \dots, 1)^T$ 

rhs\_filename for the right-hand side vector

The PLAIN and Matrix Market formats are supported for rhs\_filename. test1f.F is the Fortran version of test1.c.

#### 2.4.2 test2

Usage: test2 m n matrix\_type solution\_filename rhistory\_filename [options]

This program solves the linear equation Ax = b, where the coefficient matrix A of size mn is a discretized two dimensional Laplacian using the five point central difference scheme, with the coefficient matrix in the storage format specified by matrix\_type and the solver specified by options. It outputs the solution to solution\_filename in the extended Matrix Market format and the residual history to

rhistory\_filename in the PLAIN format. The right-hand side vector b is set such that the values of the elements of the solution x are 1. The values m and n represent the numbers of grid points in each dimension. test2f.F90 is the Fortran 90 version of test2.c.

#### 2.4.3 test2b

Usage: test2b m n matrix\_type solution\_filename rhistory\_filename [options]

This program solves the linear equation Ax = b, where the coefficient matrix A of size mn is a discretized two dimensional Laplacian using the nine point central difference scheme, with the coefficient matrix in the storage format specified by matrix\_type and the solver specified by options. It outputs the solution to solution\_filename in the extended Matrix Market format and the residual history to rhistory\_filename in the PLAIN format. The right-hand side vector b is set such that the values of the elements of the solution x are 1. The values m and n represent the numbers of grid points in each dimension.

#### 2.4.4 test3

Usage: test3 1 m n matrix\_type solution\_filename rhistory\_filename [options]

This program solves the linear equation Ax = b, where the coefficient matrix A of size lmn is a discretized three dimensional Laplacian using the seven point central difference scheme, with the coefficient matrix in the storage format specified by matrix\_type and the solver specified by options. It outputs the solution to solution\_filename in the extended Matrix Market format and the residual history to rhistory\_filename in the PLAIN format. The right-hand side vector b is set such that the values of the elements of the solution x are 1. The values 1, m and n represent the numbers of grid points in each dimension.

#### 2.4.5 test3b

Usage: test3b 1 m n matrix\_type solution\_filename rhistory\_filename [options]

This program solves the linear equation Ax = b, where the coefficient matrix A of size lmn is a discretized three dimensional Laplacian using the twenty-seven point central difference scheme, with the coefficient matrix in the storage format specified by matrix\_type and the solver specified by options. It outputs the solution to solution\_filename in the extended Matrix Market format and the residual history to rhistory\_filename in the PLAIN format. The right-hand side vector b is set such that the values of the elements of the solution x are 1. The values 1, m and m represent the numbers of grid points in each dimension.

#### 2.4.6 test3c

Usage: test3c 1 m n step [options]

This program solves the linear equation Ax = b for step steps, where the coefficient matrix A of size lmn is a discretized three dimensional Laplacian using the seven point central difference scheme, with the coefficient matrix in the CSR format and the solver specified by options. The right-hand side vector b is set such that the values of the elements of the solution x are 1. The values of the elements of the matrix and the right-hand side vector are updated at every step. The values 1, m and m represent the numbers of grid points in each dimension.

#### 2.4.7 test4

This program solves the linear equation Ax = b with a specified solver and a preconditioner, where A is a tridiagonal matrix

$$\begin{pmatrix}
2 & -1 & & & & \\
-1 & 2 & -1 & & & & \\
& \ddots & \ddots & \ddots & & \\
& & -1 & 2 & -1 \\
& & & -1 & 2
\end{pmatrix}$$

of size 12. The right-hand side vector b is set such that the values of the elements of the solution x are 1. test4f.F is the Fortran version of test4.c.

#### 2.4.8 test5

Usage: test5 n gamma [options]

This program solves a linear equation Ax = b, where A is a Toeplitz matrix

$$\begin{pmatrix}
2 & 1 & & & & \\
0 & 2 & 1 & & & \\
\gamma & 0 & 2 & 1 & & \\
& \ddots & \ddots & \ddots & \ddots & \\
& & \gamma & 0 & 2 & 1 \\
& & & \gamma & 0 & 2
\end{pmatrix}$$

of size n, with the solver specified by options. Note that the right-hand vector is set such that the values of the elements of the solution x are 1.

#### 2.4.9 test6

Usage: test6 m n

test6.c is the array version of test2.c. This program solves the linear equation Ax = b using the direct method, where the coefficient matrix A of size mn is a discretized two dimensional Laplacian using the five point central difference scheme. The right-hand side vector b is set such that the values of the elements of the solution x are 1. The values m and n represent the numbers of grid points in each dimension. test6f.F90 is the Fortran 90 version of test6.c.

#### 2.4.10 test7

Usage: test7

This program show examples of complex arithmetic. test7f.F is the Fortran version of test7.c.

### **2.4.11** etest1

Usage: etest1 matrix\_filename evector\_filename rhistory\_filename [options]

This program inputs the matrix data from matrix\_filename and solves the standard eigenvalue problem  $Ax = \lambda x$  with the solver specified by options. It outputs the specified eigenvalue to the standard output, the associated eigenvector to evector\_filename in the extended Matrix Market format, and the residual history to rhistory\_filename in the PLAIN format. Both the Matrix Market format and the Harwell-Boeing format are supported for the matrix filename. etest1f.F is the Fortran version of etest1.c. See etest5 for obtaining multiple eigenpairs.

#### 2.4.12 getest1

Usage: getest1 matrix\_a\_filename matrix\_b\_filename evector\_filename rhistory\_filename [options]

This program inputs the matrix data from matrix\_a\_filename and matrix\_b\_filename, and solves the generalized eigenvalue problem  $Ax = \lambda Bx$  with the solver specified by options. It outputs the specified eigenvalue to the standard output, the associated eigenvector to evector\_filename in the extended Matrix Market format, and the residual history to rhistory\_filename in the PLAIN format. Both the Matrix Market format and the Harwell-Boeing format are supported for the matrix filenames. See getest5 for obtaining multiple eigenpairs.

#### 2.4.13 etest2

Usage: etest2 m n matrix\_type evector\_filename rhistory\_filename [options]

This program solves the eigenvalue problem  $Ax = \lambda x$ , where the coefficient matrix A of size mn is a discretized two dimensional Laplacian using the five point central difference scheme, with the coefficient matrix in the storage format specified by matrix\_type and the solver specified by options. It outputs the specified eigenvalue to the standard output, the associated eigenvector to evector\_filename in the extended Matrix Market format, and the residual history to rhistory\_filename in the PLAIN format. The values m and n represent the numbers of grid points in each dimension.

#### 2.4.14 etest3

Usage: etest3 1 m n matrix\_type evector\_filename rhistory\_filename [options]

This program solves the eigenvalue problem  $Ax = \lambda x$ , where the coefficient matrix A of size lmn is a discretized three dimensional Laplacian using the seven point central difference scheme, with the coefficient matrix in the storage format specified by  $\mathtt{matrix\_type}$  and the solver specified by  $\mathtt{options}$ . It outputs the specified eigenvalue to the standard output, the associated eigenvector to  $\mathtt{evector\_filename}$  in the extended Matrix Market format, and the residual history to  $\mathtt{rhistory\_filename}$  in the PLAIN format. The values 1,  $\mathtt{m}$  and  $\mathtt{n}$  represent the numbers of grid points in each dimension. See  $\mathtt{etest6}$  for obtaining multiple eigenpairs.

#### 2.4.15 etest4

Usage: etest4 n [options]

This program solves the eigenvalue problem  $Ax = \lambda x$  with a specified solver, where A is a tridiagonal matrix

$$A = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

of size  $n \times n$ . etest4f.F is the Fortran version of etest4.c.

#### 2.4.16 etest5

Usage: etest5 matrix\_filename evalues\_filename evectors\_filename residuals\_filename iters\_filename [options]

This program inputs the matrix data from matrix\_filename and solves the standard eigenvalue problem  $Ax = \lambda x$  with the solver specified by options. It outputs the specified number of eigenvalues, the number of which is given by option -ss, to evalues\_filename and the associated eigenvectors, residual norms, and numbers of iterations to

evectors\_filename, residuals\_filename, and iters\_filename respectively in the extended Matrix Market format. Both the Matrix Market format and the Harwell-Boeing format are supported for the matrix filename.

#### 2.4.17 getest5

Usage: getest5 matrix\_a\_filename matrix\_b\_filename evalues\_filename evectors\_filename residuals\_filename iters\_filename [options]

This program inputs the matrix data from matrix\_a\_filename and matrix\_b\_filename, and solves the generalized eigenvalue problem  $Ax = \lambda Bx$  with the solver specified by options. It outputs the specified number of eigenvalues, the number of which is given by option -ss, to evalues\_filename and the associated eigenvectors, residual norms, and numbers of iterations to

evectors\_filename, residuals\_filename, and iters\_filename respectively in the extended Matrix Market format. Both the Matrix Market format and the Harwell-Boeing format are supported for the matrix filenames.

#### 2.4.18 etest6

Usage: etest6 l m n matrix\_type evalues\_filename evectors\_filename residuals\_filename
 iters\_filename [options]

This program solves the eigenvalue problem  $Ax = \lambda x$ , where the coefficient matrix A of size lmn is a discretized three dimensional Laplacian using the seven point central difference scheme, with the coefficient matrix in the storage format specified by matrix\_type and the solver specified by options. It outputs the specified number of eigenvalues, the number of which is given by option -ss, to evalues\_filename and the associated eigenvectors and residual norms to evectors\_filename, residuals\_filename, and iters\_filename respectively in the extended Matrix Market format. The values 1, m and n represent the numbers of grid points in each dimension.

#### 2.4.19 etest7

Usage: etest7 m n

etest7.c is the array version of etest2.c. This program solves the eigenvalue problem  $Ax = \lambda x$  using the QR algorithm, where the coefficient matrix A of size mn is a discretized two dimensional Laplacian using the five point central difference scheme. The values m and n represent the numbers of grid points in each dimension.

#### 2.4.20 spmvtest1

Usage: spmvtest1 n iter [matrix\_type]

This program computes the matrix-vector multiply of a discretized one dimensional Laplacian

$$\begin{pmatrix}
2 & -1 & & & & \\
-1 & 2 & -1 & & & & \\
& \ddots & \ddots & \ddots & & \\
& & -1 & 2 & -1 \\
& & & -1 & 2
\end{pmatrix}$$

of size n using the three point central difference scheme and a vector  $(1, ..., 1)^T$ . The FLOPS performance is measured as the average of iter iterations. If necessary, one of the following values can be specified by matrix\_type:

0 Measure the performance for the available matrix storage formats

1-11 The number of the matrix storage format

#### 2.4.21 spmvtest2

Usage: spmvtest2 m n iter [matrix\_type]

This program computes the matrix-vector multiply of a discretized two dimensional Laplacian of size mn using the five point central difference scheme and a vector  $(1, ..., 1)^T$ . The FLOPS performance is measured as the average of iter iterations. If necessary, one of the following values can be specified by matrix\_type:

0 Measure the performance for the available matrix storage formats

1-11 The number of the matrix storage format

The values m and n represent the numbers of grid points in each dimension.

#### 2.4.22 spmvtest2b

Usage: spmvtest2b m n iter [matrix\_type]

This program computes the matrix-vector multiply of a discretized two dimensional Laplacian of size mn using the nine point central difference scheme and a vector  $(1, ..., 1)^T$ . The FLOPS performance is measured as the average of iter iterations. If necessary, one of the following values can be specified by matrix\_type:

0 Measure the performance for the available matrix storage formats

1-11 The number of the matrix storage format

The values **m** and **n** represent the numbers of grid points in each dimension.

### 2.4.23 spmvtest3

Usage: spmvtest3 1 m n iter [matrix\_type]

This program computes the matrix-vector multiply of a discretized three dimensional Laplacian of size lmn using the seven point central difference scheme and a vector  $(1, ..., 1)^T$ . The values 1, m and n represent the numbers of grid points in each dimension. The FLOPS performance is measured as the average of iter iterations. If necessary, one of the following values can be specified by matrix\_type:

0 Measure the performance for the available matrix storage formats

1-11 The number of the matrix storage format

### 2.4.24 spmvtest3b

Usage: spmvtest3b 1 m n iter [matrix\_type]

This program computes the matrix-vector multiply of a discretized three dimensional Laplacian of size lmn using the twenty-seven point central difference scheme and a vector  $(1, ..., 1)^T$ . The values 1, m and n represent the numbers of grid points in each dimension. The FLOPS performance is measured as the average of iter iterations. If necessary, one of the following values can be specified by matrix\_type:

1-11

The number of the matrix storage format

## 2.4.25 spmvtest4

Usage: spmvtest4 matrix\_filename\_list iter [block]

This program inputs the matrix data from the files listed in matrix\_filename\_list, and computes the multiplies of matrices in available matrix storage formats and a vector  $(1, ..., 1)^T$ . The FLOPS performance is measured as the average of iter iterations. Both the Matrix Market format and the Harwell-Boeing format are supported for the matrix filenames. If necessary, the block size of the BSR and BSC formats can be specified by block.

### 2.4.26 spmvtest5

Usage: spmvtest5 matrix\_filename matrix\_type iter [block]

This program inputs the matrix data from matrix\_filename and compute the multiply of the matrix with matrix\_type and a vector  $(1, ..., 1)^T$ . The FLOPS performance is measured as the average of iter iterations. Both the Matrix Market format and the Harwell-Boeing format are supported for matrix\_filename. If necessary, the block size of the BSR and BSC formats can be specified by block.

#### 2.5 Limitations

The current version has the following limitations:

- Matrix storage formats
  - The VBR format does not support the multiprocessing environment.
  - The SA-AMG preconditioner supports only the CSR format.
  - In the multiprocessing environment, the CSR is the only accepted format for user defined arrays.
- Double-double (quadruple) precision operations (see Section 4)
  - The Jacobi, Gauss-Seidel, SOR, IDR(s), COCG, and COCR methods do not support the double-double precision operations.
  - The eigensolvers do not support the double-double precision operations.
  - The Jacobi, Gauss-Seidel and SOR methods in the hybrid preconditioner do not support the double-double precision operations.
  - The I+S and SA-AMG preconditioners do not support the double-double precision operations.

#### Preconditioners

- The algorithm of the ILU(k) preconditioner is based on the localized ILU preconditioning[36], which factorizes the block diagonal elements in parallel. Note that the convergence behavior approaches to that of the Jacobi preconditioner as the number of threads or processes increases.
- If a preconditioner other than the Jacobi or SSOR is selected and matrix A is not in the CSR format, a new matrix is created in the CSR format for preconditioning.
- The SA-AMG preconditioner does not support the BiCG method for unsymmetric matrices.
- The SA-AMG preconditioner does not support multithreading.
- The assembly of the matrices in the SAINV preconditioner is not parallelized.
- The user defined preconditioner cannot be used.

## 3 Basic Operations

This section describes how to use the library. A program requires the following statements:

- Initialization
- Matrix creation
- Vector creation
- Solver creation
- Value assignment for matrices and vectors
- Solver assignment
- Solver execution
- Finalization

In addition, it must include one of the following compiler directives:

```
• C #include "lis.h"
```

• Fortran #include "lisf.h"

When Lis is installed in (\$INSTALLDIR), lis.h and lisf.h are located in (\$INSTALLDIR)/include.

### 3.1 Initializing and Finalizing

The functions for initializing and finalizing the execution environment must be called at the top and bottom of the program, respectively, as follows:

```
1: #include "lis.h"
2: LIS_INT main(LIS_INT argc, char* argv[])
3: {
4: lis_initialize(&argc, &argv);
5: ...
6: lis_finalize();
7: }
```

```
Fortran

1: #include "lisf.h"

2: call lis_initialize(ierr)

3: ...

4: call lis_finalize(ierr)
```

#### Initializing

For initializing, the following functions are used:

- C LIS\_INT lis\_initialize(LIS\_INT\* argc, char\*\* argv[])
- Fortran subroutine lis\_initialize(LIS\_INTEGER ierr)

This function initializes the MPI execution environment, and specifies the options on the command line. The default type of the integer in the C programs is LIS\_INT, which is equivalent to int. If the preprossor macro \_LONG\_\_LONG is defined, it is replaced with long long int. The default type of the integer in the Fortran programs is LIS\_INTEGER, which is equivalent to integer. If the preprocessor

macro LONG\_LONG is defined, it is replaced with integer\*8.

#### **Finalizing**

For finalizing, the following functions are used:

- C LIS\_INT lis\_finalize()
- Fortran subroutine lis\_finalize(LIS\_INTEGER ierr)

#### 3.2 Operating Vectors

Assume that the size of vector v is  $global\_n$ , and the size of each partial vector stored on nprocs processing elements is  $local\_n$ . If  $global\_n$  is divisible, then  $local\_n$  is equal to  $global\_n / nprocs$ . For example, when vector v is stored on two processing elements, as shown in Equation (3.1),  $global\_n$  and  $local\_n$  are 4 and 2, respectively.

$$v = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 3 \end{pmatrix} \text{ PE0}$$
PE1 (3.1)

In the case of creating vector v in Equation (3.1), vector v itself is created for the serial and multithreaded environments, while the partial vectors are created and stored on a given number of processing elements for the multiprocessing environment.

Programs to create vector v are as follows, where the number of processing elements for the multiprocessing environment is assumed to be two:

```
C (for serial and multithreaded environments)

1: LIS_INT i,n;
2: LIS_VECTOR v;
3: n = 4;
4: lis_vector_create(0,&v);
5: lis_vector_set_size(v,0,n); /* or lis_vector_set_size(v,n,0); */
6:
7: for(i=0;i<n;i++)
8: {
9: lis_vector_set_value(LIS_INS_VALUE,i,(double)i,v);
10: }
```

```
Fortran (for serial and multithreaded environments)

1: LIS_INTEGER i,n

2: LIS_VECTOR v

3: n = 4

4: call lis_vector_create(0,v,ierr)

5: call lis_vector_set_size(v,0,n,ierr)

6:

7: do i=1,n

9: call lis_vector_set_value(LIS_INS_VALUE,i,DBLE(i),v,ierr)

10: enddo
```

```
Fortran (for multiprocessing environment)

1: LIS_INTEGER i,n,is,ie

2: LIS_VECTOR v

3: n = 4

4: call lis_vector_create(MPI_COMM_WORLD,v,ierr)

5: call lis_vector_set_size(v,0,n,ierr)

6: call lis_vector_get_range(v,is,ie,ierr)

7: do i=is,ie-1

8: call lis_vector_set_value(LIS_INS_VALUE,i,DBLE(i),v,ierr);

9: enddo
```

#### **Creating Vectors**

To create vector v, the following functions are used:

- C LIS\_INT lis\_vector\_create(LIS\_Comm comm, LIS\_VECTOR \*v)
- Fortran subroutine lis\_vector\_create(LIS\_Comm comm, LIS\_VECTOR v, LIS\_INTEGER ierr)

For the example program above, comm must be replaced with the MPI communicator. For the serial and multithreaded environments, the value of comm is ignored.

#### **Assigning Sizes**

To assign a size to vector v, the following functions are used:

- C LIS\_INT lis\_vector\_set\_size(LIS\_VECTOR v, LIS\_INT local\_n, LIS\_INT global\_n)
- Fortran subroutine lis\_vector\_set\_size(LIS\_VECTOR v, LIS\_INTEGER local\_n, LIS\_INTEGER global\_n, LIS\_INTEGER ierr)

Either  $local\_n$  or  $global\_n$  must be provided.

For the serial and multithreaded environments,  $local_n$  is equal to  $global_n$ . Therefore, both  $lis_vector_set_size(v,n,0)$  and  $lis_vector_set_size(v,0,n)$  create a vector of size n.

For the multiprocessing environment,  $lis_{vector_set_size(v,n,0)}$  creates a partial vector of size n on each processing element. On the other hand,  $lis_{vector_set_size(v,0,n)}$  creates a partial vector of size  $m_p$  on processing element p. The values of  $m_p$  are determined by the library.

#### **Assigning Values**

To assign a value to the i-th element of vector v, the following functions are used:

- C LIS\_INT lis\_vector\_set\_value(LIS\_INT flag, LIS\_INT i, LIS\_SCALAR value, LIS\_VECTOR v)
- Fortran subroutine lis\_vector\_set\_value(LIS\_INTEGER flag, LIS\_INTEGER i, LIS\_SCALAR value, LIS\_VECTOR v, LIS\_INTEGER ierr)

For the multiprocessing environment, the i-th row of the global vector must be specified. Either

 $LIS_{INS_{VALUE}} : v[i] = value, or$ 

 $\texttt{LIS\_ADD\_VALUE} \, : \, v[i] = v[i] + value$ 

must be provided for flag.

#### **Duplicating Vectors**

To create a vector that has the same information as the existing vector, the following functions are used:

- C LIS\_INT lis\_vector\_duplicate(LIS\_VECTOR vin, LIS\_VECTOR \*vout)
- Fortran subroutine lis\_vector\_duplicate(LIS\_VECTOR vin, LIS\_VECTOR vout, LIS\_INTEGER ierr)

This function does not copy the values of the vector. To copy the values as well, the following functions must be called after the above functions:

- C LIS\_INT lis\_vector\_copy(LIS\_VECTOR vsrc, LIS\_VECTOR vdst)
- Fortran subroutine lis\_vector\_copy(LIS\_VECTOR vsrc, LIS\_VECTOR vdst, LIS\_INTEGER ierr)

#### **Destroying Vectors**

To destroy the vector, the following functions are used:

- C LIS\_INT lis\_vector\_destroy(LIS\_VECTOR v)
- Fortran subroutine lis\_vector\_destroy(LIS\_VECTOR v, LIS\_INTEGER ierr)

### 3.3 Operating Matrices

Assume that the size of matrix A is  $global\_n \times global\_n$ , and that the size of each row block of matrix A stored on nprocs processing elements is  $local\_n \times global\_n$ . If  $global\_n$  is divisible, then  $local\_n$  is equal to  $global\_n / nprocs$ . For example, when the row block of matrix A is stored on two processing elements, as shown in Equation (3.2),  $global\_n$  and  $local\_n$  are 4 and 2, respectively.

$$A = \begin{pmatrix} 2 & 1 & & \\ 1 & 2 & 1 & & \\ \hline & 1 & 2 & 1 & \\ & & 1 & 2 & \end{pmatrix} \text{ PE0}$$
(3.2)

A matrix in a specific storage format can be created in one of the following three ways:

### Method 1: Define Arrays in a Specific Storage Format with Library Functions

For creating matrix A in Equation (3.2) in the CSR format, matrix A itself is created for the serial and multithreaded environments, while partial matrices are created and stored on the given number of processing elements for the multiprocessing environment.

Programs to create matrix A in the CSR format are as follows, where the number of processing elements for the multiprocessing environment is assumed to be two:

```
— C (for serial and multithreaded environments) —
 1: LIS_INT i,n;
2: LIS_MATRIX A;
3: n = 4;
 4: lis_matrix_create(0,&A);
                                            /* or lis_matrix_set_size(A,n,0); */
5: lis_matrix_set_size(A,0,n);
 6: for(i=0;i<n;i++) {
        if( i>0 ) lis_matrix_set_value(LIS_INS_VALUE,i,i-1,1.0,A);
7:
        if( i<n-1 ) lis_matrix_set_value(LIS_INS_VALUE,i,i+1,1.0,A);</pre>
8:
9:
        lis_matrix_set_value(LIS_INS_VALUE,i,i,2.0,A);
10: }
11: lis_matrix_set_type(A,LIS_MATRIX_CSR);
12: lis_matrix_assemble(A);
```

```
- C (for multiprocessing environment) -
1: LIS_INT i,n,gn,is,ie;
2: LIS_MATRIX A;
3: gn = 4;
                                              /* or n=2 */
4: lis_matrix_create(MPI_COMM_WORLD,&A);
5: lis_matrix_set_size(A,0,gn);
                                              /* lis_matrix_set_size(A,n,0); */
6: lis_matrix_get_size(A,&n,&gn);
7: lis_matrix_get_range(A,&is,&ie);
8: for(i=is;i<ie;i++) {
9:
        if( i>0 ) lis_matrix_set_value(LIS_INS_VALUE,i,i-1,1.0,A);
        if( i<gn-1 ) lis_matrix_set_value(LIS_INS_VALUE,i,i+1,1.0,A);</pre>
10:
        lis_matrix_set_value(LIS_INS_VALUE,i,i,2.0,A);
11:
12: }
13: lis_matrix_set_type(A,LIS_MATRIX_CSR);
14: lis_matrix_assemble(A);
```

```
    Fortran (for multiprocessing environment) -

 1: LIS_INTEGER i,n,gn,is,ie
2: LIS_MATRIX A
3: gn = 4
4: call lis_matrix_create(MPI_COMM_WORLD,A,ierr)
5: call lis_matrix_set_size(A,0,gn,ierr)
6: call lis_matrix_get_size(A,n,gn,ierr)
7: call lis_matrix_get_range(A,is,ie,ierr)
8: do i=is,ie-1
        if( i>1 ) call lis_matrix_set_value(LIS_INS_VALUE,i,i-1,1.0d0,A,ierr)
10:
        if( i<gn ) call lis_matrix_set_value(LIS_INS_VALUE,i,i+1,1.0d0,A,ierr)</pre>
        call lis_matrix_set_value(LIS_INS_VALUE,i,i,2.0d0,A,ierr)
11:
12: enddo
13: call lis_matrix_set_type(A,LIS_MATRIX_CSR,ierr)
14: call lis_matrix_assemble(A,ierr)
```

#### **Creating Matrices**

To create matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_create(LIS\_Comm comm, LIS\_MATRIX \*A)
- Fortran subroutine lis\_matrix\_create(LIS\_Comm comm, LIS\_MATRIX A, LIS\_INTEGER ierr)

comm must be replaced with the MPI communicator. For the serial and multithreaded environments, the value of comm is ignored.

#### Assigning Sizes

To assign a size to matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_size(LIS\_MATRIX A, LIS\_INT local\_n, LIS\_INT global\_n)
- Fortran subroutine lis\_matrix\_set\_size(LIS\_MATRIX A, LIS\_INTEGER local\_n, LIS\_INTEGER global\_n, LIS\_INTEGER ierr)

Either  $local_n$  or  $global_n$  must be provided.

For the serial and multithreaded environments,  $local_n$  is equal to  $global_n$ . Therefore, both  $lis_matrix_set_size(A,n,0)$  and  $lis_matrix_set_size(A,0,n)$  create a matrix of size  $n \times n$ .

For the multiprocessing environment,  $lis_matrix_set_size(A,n,0)$  creates a partial matrix of size  $n \times N$  on each processing element, where N is the total sum of n. On the other hand,  $lis_matrix_set_size(A,0,n)$  creates a partial matrix of size  $m_p \times n$  on processing element p. The values of  $m_p$  are determined by the library.

#### **Assigning Values**

To assign a value to the element at the i-th row and the j-th column of matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_value(LIS\_INT flag, LIS\_INT i, LIS\_INT j, LIS\_SCALAR value, LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_value(LIS\_INTEGER flag, LIS\_INTEGER i, LIS\_INTEGER j, LIS\_SCALAR value, LIS\_MATRIX A, LIS\_INTEGER ierr)

For the multiprocessing environment, the i-th row and the j-th column of the global matrix must be specified. Either

```
\begin{split} & \texttt{LIS\_INS\_VALUE} \,:\, A(i,j) = value, \, \text{or} \\ & \texttt{LIS\_ADD\_VALUE} \,:\, A(i,j) = A(i,j) + value \end{split}
```

must be provided for the parameter flag.

#### **Assigning Storage Formats**

To assign a storage format to matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_type(LIS\_MATRIX A, LIS\_INT matrix\_type)
- Fortran subroutine lis\_matrix\_set\_type(LIS\_MATRIX A, LIS\_INTEGER matrix\_type, LIS\_INTEGER ierr)

where matrix\_type is LIS\_MATRIX\_CSR when the matrix is created. The following storage formats are supported:

Storage format		matrix_type
Compressed Sparse Row	(CSR)	{LIS_MATRIX_CSR 1}
Compressed Sparse Column	(CSC)	{LIS_MATRIX_CSC 2}
Modified Compressed Sparse Row	(MSR)	{LIS_MATRIX_MSR 3}
Diagonal	(DIA)	{LIS_MATRIX_DIA 4}
Ellpack-Itpack Generalized Diagonal	(ELL)	{LIS_MATRIX_ELL 5}
Jagged Diagonal	(JAD)	{LIS_MATRIX_JAD 6}
Block Sparse Row	(BSR)	{LIS_MATRIX_BSR 7}
Block Sparse Column	(BSC)	{LIS_MATRIX_BSC 8}
Variable Block Row	(VBR)	{LIS_MATRIX_VBR 9}
Coordinate	(COO)	{LIS_MATRIX_COO 10}
Dense	(DNS)	{LIS_MATRIX_DNS 11}

#### **Assembling Matrices**

After assigning values and storage formats, the following functions must be called:

- C LIS\_INT lis\_matrix\_assemble(LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_assemble(LIS\_MATRIX A, LIS\_INTEGER ierr)

 $\verb|lis_matrix_assemble| assembles A into the storage format specified by \verb|lis_matrix_set_type|.$ 

## **Destroying Matrices**

To destroy the matrix, the following functions are used:

- C LIS\_INT lis\_matrix\_destroy(LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_destroy(LIS\_MATRIX A, LIS\_INTEGER ierr)

#### Method 2: Define Arrays in a Specific Storage Format Directly

For creating matrix A in Equation (3.2) in the CSR format, matrix A itself is created for the serial and multithreaded environments, while the partial matrices are created and stored on the given number of processing elements for the multiprocessing environment.

Programs to create matrix A in the CSR format are as follows, where the number of processing elements for the multiprocessing environment is assumed to be two:

```
— C (for serial and multithreaded environments) –
 1: LIS_INT i,k,n,nnz;
2: LIS_INT *ptr,*index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 4; nnz = 10; k = 0;
6: lis_matrix_malloc_csr(n,nnz,&ptr,&index,&value);
7: lis_matrix_create(0,&A);
                                           /* or lis_matrix_set_size(A,n,0); */
8: lis_matrix_set_size(A,0,n);
9:
10: for(i=0;i<n;i++)
11: {
12:
        if( i>0 ) {index[k] = i-1; value[k] = 1; k++;}
13:
        index[k] = i; value[k] = 2; k++;
14:
        if( i < n-1 ) {index[k] = i+1; value[k] = 1; k++;}
15:
        ptr[i+1] = k;
16: }
17: ptr[0] = 0;
18: lis_matrix_set_csr(nnz,ptr,index,value,A);
19: lis_matrix_assemble(A);
```

```
— C (for multiprocessing environment) —
1: LIS_INT i,k,n,nnz,is,ie;
2: LIS_INT *ptr,*index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 2; nnz = 5; k = 0;
6: lis_matrix_malloc_csr(n,nnz,&ptr,&index,&value);
7: lis_matrix_create(MPI_COMM_WORLD,&A);
8: lis_matrix_set_size(A,n,0);
9: lis_matrix_get_range(A,&is,&ie);
10: for(i=is;i<ie;i++)</pre>
11: {
12:
        if( i>0 ) {index[k] = i-1; value[k] = 1; k++;}
13:
        index[k] = i; value[k] = 2; k++;
14:
        if( i < n-1 ) {index[k] = i+1; value[k] = 1; k++;}
15:
        ptr[i-is+1] = k;
16: }
17: ptr[0] = 0;
18: lis_matrix_set_csr(nnz,ptr,index,value,A);
19: lis_matrix_assemble(A);
```

#### **Associating Arrays**

To associate the arrays in the CSR format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_csr(LIS\_INT nnz, LIS\_INT ptr[], LIS\_INT index[], LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_csr(LIS\_INTEGER nnz, LIS\_INTEGER ptr(), LIS\_INTEGER index(), LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

#### Method 3: Read Matrix and Vector Data from External Files

Programs to read matrix A in Equation (3.2) in the CSR format and vector b in Equation (3.1) from an external file are as follows:

```
C (for serial, multithreaded and multiprocessing environments)

1: LIS_MATRIX A;
2: LIS_VECTOR b,x;
3: lis_matrix_create(LIS_COMM_WORLD,&A);
4: lis_vector_create(LIS_COMM_WORLD,&b);
5: lis_vector_create(LIS_COMM_WORLD,&x);
6: lis_matrix_set_type(A,LIS_MATRIX_CSR);
7: lis_input(A,b,x,"matvec.mtx");
```

```
Fortran (for serial, multithreaded and multiprocessing environments)

1: LIS_MATRIX A

2: LIS_VECTOR b,x

3: call lis_matrix_create(LIS_COMM_WORLD,A,ierr)

4: call lis_vector_create(LIS_COMM_WORLD,b,ierr)

5: call lis_vector_create(LIS_COMM_WORLD,x,ierr)

6: call lis_matrix_set_type(A,LIS_MATRIX_CSR,ierr)

7: call lis_input(A,b,x,'matvec.mtx',ierr)
```

The content of the destination file matvec.mtx is:

```
%%MatrixMarket matrix coordinate real general
4 4 10 1 0
1 2 1.0e+00
1 1 2.0e+00
2 3 1.0e+00
2 1 1.0e+00
2 2 2.0e+00
3 4 1.0e+00
3 2 1.0e+00
3 3 2.0e+00
4 4 2.0e+00
4 3 1.0e+00
1 0.0e+00
2 1.0e+00
3 2.0e+00
4 3.0e+00
```

#### Reading from External Files

To input the matrix data for A from an external file, the following functions are used:

```
• C LIS_INT lis_input_matrix(LIS_MATRIX A, char *filename)
```

```
• Fortran subroutine lis_input(LIS_MATRIX A, character filename, LIS_INTEGER ierr)
```

filename must be replaced with the file path. The following file formats are supported:

- The Matrix Market format
- The Harwell-Boeing format

To read the data for matrix A and vectors b and x from external files, the following functions are used:

- C LIS\_INT lis\_input(LIS\_MATRIX A, LIS\_VECTOR b, LIS\_VECTOR x, char \*filename)
- Fortran subroutine lis\_input(LIS\_MATRIX A, LIS\_VECTOR b, LIS\_VECTOR x, character filename, LIS\_INTEGER ierr)

filename must be replaced with the file path. The following file formats are supported:

- The Extended Matrix Market format (extended to allow vector data)
- The Harwell-Boeing format

### 3.4 Solving Linear Equations

A program to solve the linear equation Ax = b with a specified solver is as follows:

```
C (for serial, multithreaded and multiprocessing environments)

1: LIS_MATRIX A;
2: LIS_VECTOR b,x;
3: LIS_SOLVER solver;
4:
5: /* Create matrix and vector */
6:
7: lis_solver_create(&solver);
8: lis_solver_set_option("-i bicg -p none",solver);
9: lis_solver_set_option("-tol 1.0e-12",solver);
10: lis_solve(A,b,x,solver);
```

```
Fortran (for serial, multithreaded and multiprocessing environments)

1: LIS_MATRIX A

2: LIS_VECTOR b,x

3: LIS_SOLVER solver

4:

5: /* Create matrix and vector */

6:

7: call lis_solver_create(solver,ierr)

8: call lis_solver_set_option('-i bicg -p none',solver,ierr)

9: call lis_solver_set_option('-tol 1.0e-12',solver,ierr)

10: call lis_solve(A,b,x,solver,ierr)
```

#### Creating Solvers

To create a solver, the following functions are used:

- C LIS\_INT lis\_solver\_create(LIS\_SOLVER \*solver)
- Fortran subroutine lis\_solver\_create(LIS\_SOLVER solver, LIS\_INTEGER ierr)

#### **Specifying Options**

To specify options, the following functions are used:

- C LIS\_INT lis\_solver\_set\_option(char \*text, LIS\_SOLVER solver)
- Fortran subroutine lis\_solver\_set\_option(character text, LIS\_SOLVER solver, LIS\_INTEGER ierr)

or

• C LIS\_INT lis\_solver\_set\_optionC(LIS\_SOLVER solver)

• Fortran subroutine lis\_solver\_set\_optionC(LIS\_SOLVER solver, LIS\_INTEGER ierr)

<code>lis\_solver\_set\_optionC</code> is a function that sets the options specified on the command line, and passes them to <code>solver</code> when the program is run.

The table below shows the available command line options, where  $-i \{cg|1\}$  means -i cg or -i 1 and -maxiter [1000] indicates that -maxiter defaults to 1,000.

Options for Linear Solvers (Default: -i bicg)

Options for Linear Solvers (Default: -i bicg)					
Solver	Option	Auxiliary Options			
CG	-i {cg 1}				
$\operatorname{BiCG}$	-i {bicg 2}				
CGS	-i {cgs 3}				
BiCGSTAB	-i {bicgstab 4}				
BiCGSTAB(1)	-i {bicgstabl 5}	-ell [2]	The degree $l$		
GPBiCG	-i {gpbicg 6}				
TFQMR	-i {tfqmr 7}				
Orthomin(m)	-i {orthomin 8}	-restart [40]	The restart value $m$		
GMRES(m)	-i {gmres 9}	-restart [40]	The restart value $m$		
Jacobi	-i {jacobi 10}				
Gauss-Seidel	-i {gs 11}				
SOR	-i {sor 12}	-omega [1.9]	The relaxation coefficient		
			$\omega \ (0 < \omega < 2)$		
BiCGSafe	-i {bicgsafe 13}				
$\operatorname{CR}$	-i {cr 14}				
$\operatorname{BiCR}$	-i {bicr 15}				
CRS	-i {crs 16}				
BiCRSTAB	-i {bicrstab 17}				
GPBiCR	-i {gpbicr 18}				
BiCRSafe	-i {bicrsafe 19}				
FGMRES(m)	-i {fgmres 20}	-restart [40]	The restart value $m$		
IDR(s)	-i {idrs 21}	-irestart [2]	The restart value $s$		
IDR(1)	-i {idr1 22}				
MINRES	-i {minres 23}				
COCG	-i {cocg 24}				
COCR	-i {cocr 25}				

Options for Preconditioners (Default: -p none)

Preconditioner	Option	Auxiliary Options	
None	-p {none 0}		
Jacobi	-p {jacobi 1}		
ILU(k)	-p {ilu 2}	-ilu_fill [0]	The fill level $k$
SSOR	-p {ssor 3}	-ssor_omega [1.0]	The relaxation coefficient
			$\omega \ (0 < \omega < 2)$
Hybrid	-p {hybrid 4}	-hybrid_i [sor]	The linear solver
		-hybrid_maxiter [25]	The maximum number of iterations
		-hybrid_tol [1.0e-3]	The convergence tolerance
		-hybrid_omega [1.5]	The relaxation coefficient $\omega$
			of the SOR $(0 < \omega < 2)$
		-hybrid_ell [2]	The degree $l$ of the BiCGSTAB(1)
		-hybrid_restart [40]	The restart values
			of the GMRES and Orthomin
I+S	-p {is 5}	-is_alpha [1.0]	The parameter $\alpha$ of $I + \alpha S^{(m)}$
		-is_m [3]	The parameter $m$ of $I + \alpha S^{(m)}$
SAINV	-p {sainv 6}	-sainv_drop [0.05]	The drop criterion
SA-AMG	-p {saamg 7}	-saamg_unsym [false]	Select the unsymmetric version
			(The matrix structure must be
			symmetric)
		-saamg_theta [0.05 0.12]	The drop criterion $a_{ij}^2 \le \theta^2  a_{ii}   a_{jj} $
			(symmetric or unsymmetric)
Crout ILU	-p {iluc 8}	-iluc_drop [0.05]	The drop criterion
		-iluc_rate [5.0]	The ratio of the maximum fill-in
ILUT	-p {ilut 9}		
Additive	-adds true	-adds_iter [1]	The number of iterations
Schwarz			

## Other Options

Option				
-maxiter [1000]	The maximum number of iterations			
-tol [1.0e-12]	The convergence tolerance tol			
-tol_w [1.0]	The convergence tolerance $tol_w$			
-print [0]	The output of the residual history			
	-print {none 0}	None		
	-print {mem 1}	Save the residual history		
	-print {out 2}	Output it to the standard output		
	-print {all 3}	Save the residual history and output it		
		to the standard output		
-scale [0]	The scaling			
	(The result will overw	rite the original matrix and vectors)		
	-scale {none 0}	No scaling		
	-scale {jacobi 1}	~		
		(D represents the diagonal of $A = (a_{ij})$ )		
	-scale {symm_diag 2	2) The diagonal scaling $D^{-1/2}AD^{-1/2}x = D^{-1/2}b$		
		$(D^{-1/2}$ represents the diagonal matrix		
		with $1/\sqrt{a_{ii}}$ as the diagonal)		
-initx_zeros [1]	The behavior of the in	· ·		
	-initx_zeros {false	- 0 0		
		of the function lis_solve()		
	-initx_zeros {true	•		
-conv_cond [0]	The convergence condi			
	-conv_cond {nrm2_r	11 11 -11		
		1} $  b - Ax  _2 \le tol *   b  _2$		
	-conv_cond {nrm1_b	11 11 11 11-		
-omp_num_threads [t]	The number of threads			
	` -	mum number of threads)		
-storage [0]	The matrix storage format			
-storage_block [2]	The block size of the BSR and BSC formats			
-f [0]	The precision of the lin			
	-f {double 0}	Double precision		
	-f {quad 1}	Double-double (quadruple) precision		

## **Solving Linear Equations**

To solve the linear equation Ax = b, the following functions are used:

- C LIS\_INT lis\_solve(LIS\_MATRIX A, LIS\_VECTOR b, LIS\_VECTOR x, LIS\_SOLVER solver)
- Fortran subroutine lis\_solve(LIS\_MATRIX A, LIS\_VECTOR b, LIS\_VECTOR x, LIS\_SOLVER solver, LIS\_INTEGER ierr)

## 3.5 Solving Eigenvalue Problems

A program to solve the standard eigenvalue problem  $Ax = \lambda x$  with a specified solver is as follows:

```
C (for serial, multithreaded and multiprocessing environments)

1: LIS_MATRIX A;
2: LIS_VECTOR x;
3: LIS_REAL evalue;
4: LIS_ESOLVER esolver;
5:
6: /* Create matrix and vector */
7:
8: lis_esolver_create(&esolver);
9: lis_esolver_set_option("-e ii -i bicg -p none",esolver);
10: lis_esolver_set_option("-etol 1.0e-12 -tol 1.0e-12",esolver);
11: lis_esolve(A,x,evalue,esolver);
```

```
Fortran (for serial, multithreaded and multiprocessing environments)

1: LIS_MATRIX A

2: LIS_VECTOR x

3: LIS_REAL evalue

4: LIS_ESOLVER esolver

5:

6: /* Create matrix and vector */

7:

8: call lis_esolver_create(esolver,ierr)

9: call lis_esolver_set_option('-e ii -i bicg -p none',esolver,ierr)

10: call lis_esolver_set_option('-etol 1.0e-12 -tol 1.0e-12',esolver,ierr)

11: call lis_esolve(A,x,evalue,esolver,ierr)
```

#### Creating Eigensolvers

To create an eigensolver, the following functions are used:

- C LIS\_INT lis\_esolver\_create(LIS\_ESOLVER \*esolver)
- Fortran subroutine lis\_esolver\_create(LIS\_ESOLVER esolver, LIS\_INTEGER ierr)

#### **Specifying Options**

To specify options, the following functions are used:

- C LIS\_INT lis\_esolver\_set\_option(char \*text, LIS\_ESOLVER esolver)
- Fortran subroutine lis\_esolver\_set\_option(character text, LIS\_ESOLVER esolver, LIS\_INTEGER ierr)

or

- C LIS\_INT lis\_esolver\_set\_optionC(LIS\_ESOLVER esolver)
- Fortran subroutine lis\_esolver\_set\_optionC(LIS\_ESOLVER esolver, LIS\_INTEGER ierr)

lis\_esolver\_set\_optionC is a function that sets the options specified in the command line, and passes them to esolver when the program is run.

The table below shows the available command line options, where -e {pi|1} means -e pi or -e 1 and -emaxiter [1000] indicates that -emaxiter defaults to 1,000.

# Options for Eigensolvers (Default: -e cr)

Eigensolver	Option	Auxiliary Options	
Power	-e {pi 1}		
Inverse	-e {ii 2}	-i [bicg]	The linear solver
Rayleigh Quotient	-e {rqi 3}	-i [bicg]	The linear solver
$\overline{CG}$	-e {cg 4}	-i [cg]	The linear solver
$\operatorname{CR}$	-e {cr 5}	-i [bicg]	The linear solver
Subspace	-e {si 6}	-ss [1]	The size of the subspace
Lanczos	-e {li 7}	-ss [1]	The size of the subspace
Arnoldi	-e {ai 8}	-ss [1]	The size of the subspace
Generalized Power	-e {gpi 9}	-i [bicg]	The linear solver
Generalized Inverse	-e {gii 10}	-i [bicg]	The linear solver
Generalized Rayleigh Quotient	-e {grqi 11}	-i [bicg]	The linear solver
Generalized CG	-e {gcg 12}	-i [cg]	The linear solver
Generalized CR	-e {gcr 13}	-i [bicg]	The linear solver
Generalized Subspace	-e {gsi 14}	-ss [1]	The size of the subspace
Generalized Lanczos	-e {gli 15}	-ss [1]	The size of the subspace
Generalized Arnoldi	-e {gai 16}	-ss [1]	The size of the subspace

# ${\bf Options} \ {\bf for} \ {\bf Preconditioners} \ ({\bf Default:} \ {\tt -p} \ {\tt none})$

Preconditioner	Option	Auxiliary Options	
None	-p {none 0}		
Jacobi	-p {jacobi 1}		
ILU(k)	-p {ilu 2}	-ilu_fill [0]	The fill level $k$
SSOR	-p {ssor 3}	-ssor_omega [1.0]	The relaxation coefficient
			$\omega \ (0 < \omega < 2)$
Hybrid	-p {hybrid 4}	-hybrid_i [sor]	The linear solver
		-hybrid_maxiter [25]	The maximum number of iterations
		-hybrid_tol [1.0e-3]	The convergence tolerance
		-hybrid_omega [1.5]	The relaxation coefficient $\omega$
			of the SOR $(0 < \omega < 2)$
		-hybrid_ell [2]	The degree $l$ of the BiCGSTAB(l)
		-hybrid_restart [40]	The restart values of the GMRES
			and Orthomin
I+S	-p {is 5}	-is_alpha [1.0]	The parameter $\alpha$ of $I + \alpha S^{(m)}$
		-is_m [3]	The parameter $m$ of $I + \alpha S^{(m)}$
SAINV	-p {sainv 6}	-sainv_drop [0.05]	The drop criterion
SA-AMG	-p {saamg 7}	-saamg_unsym [false]	Select the unsymmetric version
			(The matrix structure must be symmetric)
		-saamg_theta [0.05 0.12]	The drop criterion $a_{ij}^2 \le \theta^2  a_{ii}   a_{jj} $
		-	(symmetric or unsymmetric)
Crout ILU	-p {iluc 8}	-iluc_drop [0.05]	The drop criterion
		-iluc_rate [5.0]	The ratio of the maximum fill-in
ILUT	-p {ilut 9}		
Additive Schwarz	-adds true	-adds_iter [1]	The number of iterations
Schwarz			

## Other Options

Option					
-emaxiter [1000]	The maximum number of iterations				
-etol [1.0e-12]	The convergence tolerance				
-eprint [0]	The output of the residual history				
	-eprint {none 0}	None			
	-eprint {mem 1}	Save the residual history			
	-eprint {out 2}	Output it to the standard output			
	-print {all 3}	Save the residual history and output it			
		to the standard output			
-ie [ii]	The inner eigensolver us	sed in Subspace, Lanczos, and Arnoldi			
-ige [gii]	The inner eigensolver us	sed in Generalized Subspace, Generalized Lanczos,			
	and Generalized Arnold	i			
-shift [0.0]	The amount of the real	part of the shift $\sigma$			
-shift_im [0.0]	The amount of the imag	ginary part of the shift $\sigma$			
-initx_ones [1]	The behavior of the initial vector $x_0$				
	-initx_ones {false 0	Components are given by the argument $x$			
		of the function lis_esolve()			
	-initx_ones {true 1}	All the components are set to 1			
-omp_num_threads [t]	The number of threads				
	(t represents the maxim	num number of threads)			
-estorage [0]	The matrix storage format				
-estorage_block [2]	The block size of the BSR and BSC formats				
-ef [0]	The precision of the eigensolver				
	-ef {double 0}	Double precision			
	-ef {quad 1}	Double-double (quadruple) precision			

### Solving Eigenvalue Problems

To solve the standard eigenvalue problem  $Ax = \lambda x$ , the following functions are used:

- C LIS\_INT lis\_esolve(LIS\_MATRIX A, LIS\_VECTOR x, LIS\_REAL evalue, LIS\_ESOLVER esolver)
- Fortran subroutine lis\_esolve(LIS\_MATRIX A, LIS\_VECTOR x, LIS\_REAL evalue, LIS\_ESOLVER esolver, LIS\_INTEGER ierr)

To solve the generalized eigenvalue problem  $Ax = \lambda Bx$ , the following functions are used instead:

- C LIS\_INT lis\_gesolve(LIS\_MATRIX A, LIS\_MATRIX B, LIS\_VECTOR x, LIS\_REAL evalue, LIS\_ESOLVER esolver)
- Fortran subroutine lis\_gesolve(LIS\_MATRIX A, LIS\_MATRIX B, LIS\_VECTOR x, LIS\_REAL evalue, LIS\_ESOLVER esolver, LIS\_INTEGER ierr)

## 3.6 Writing Programs

The following are the programs for solving the linear equation Ax = b, where matrix A is a tridiagonal matrix

$$\begin{pmatrix}
2 & -1 & & & & \\
-1 & 2 & -1 & & & & \\
& \ddots & \ddots & \ddots & & \\
& & -1 & 2 & -1 & \\
& & & -1 & 2
\end{pmatrix}$$

of size 12. The the right-hand side vector b is set such that the values of the elements of the solution x are 1. The programs are located in the directory lis-(\$VERSION)/test.

```
- Test program: test4.c -
 1: #include <stdio.h>
 2: #include "lis.h"
 3: main(LIS_INT argc, char *argv[])
 4: {
5:
        LIS_INT i,n,gn,is,ie,iter;
 6:
        LIS_MATRIX A;
 7:
        LIS_VECTOR b,x,u;
 8:
        LIS_SOLVER solver;
9:
        n = 12;
10:
        lis_initialize(&argc,&argv);
11:
        lis_matrix_create(LIS_COMM_WORLD,&A);
12:
        lis_matrix_set_size(A,0,n);
13:
        lis_matrix_get_size(A,&n,&gn)
14:
        lis_matrix_get_range(A,&is,&ie)
        for(i=is;i<ie;i++)</pre>
15:
16:
            if( i>0 ) lis_matrix_set_value(LIS_INS_VALUE,i,i-1,-1.0,A);
17:
18:
            if( i<gn-1 ) lis_matrix_set_value(LIS_INS_VALUE,i,i+1,-1.0,A);</pre>
19:
            lis_matrix_set_value(LIS_INS_VALUE,i,i,2.0,A);
20:
21:
        lis_matrix_set_type(A,LIS_MATRIX_CSR);
22:
        lis_matrix_assemble(A);
23:
24:
        lis_vector_duplicate(A,&u);
        lis_vector_duplicate(A,&b);
25:
26:
        lis_vector_duplicate(A,&x);
27:
        lis_vector_set_all(1.0,u);
        lis_matvec(A,u,b);
28:
29:
30:
        lis_solver_create(&solver);
31:
        lis_solver_set_optionC(solver);
32:
        lis_solve(A,b,x,solver);
        lis_solver_get_iter(solver,&iter);
33:
34:
        printf("number of iterations = %d\n",iter);
35:
        lis_vector_print(x);
        lis_matrix_destroy(A);
36:
37:
        lis_vector_destroy(u);
38:
        lis_vector_destroy(b);
39:
        lis_vector_destroy(x);
40:
        lis_solver_destroy(solver);
41:
        lis_finalize();
42:
        return 0;
43: }
}
```

```
– Test program: test4f.F –
         implicit none
 2:
3:#include "lisf.h"
 4:
         LIS_INTEGER i,n,gn,is,ie,iter,ierr
 5:
         LIS_MATRIX A
 6:
7:
         LIS_VECTOR b,x,u
         LIS_SOLVER solver
8:
9:
         n = 12
10:
         call lis_initialize(ierr)
11:
         call lis_matrix_create(LIS_COMM_WORLD,A,ierr)
12:
         call lis_matrix_set_size(A,0,n,ierr)
13:
         call lis_matrix_get_size(A,n,gn,ierr)
14:
         call lis_matrix_get_range(A,is,ie,ierr)
         do i=is,ie-1
15:
16:
           if( i>1 ) call lis_matrix_set_value(LIS_INS_VALUE,i,i-1,-1.0d0,
17:
                                                  A,ierr)
           if( i<gn ) call lis_matrix_set_value(LIS_INS_VALUE,i,i+1,-1.0d0,</pre>
18:
19:
                                                  A,ierr)
20:
           call lis_matrix_set_value(LIS_INS_VALUE,i,i,2.0d0,A,ierr)
21:
         enddo
22:
         call lis_matrix_set_type(A,LIS_MATRIX_CSR,ierr)
23:
         call lis_matrix_assemble(A,ierr)
24:
25:
         call lis_vector_duplicate(A,u,ierr)
26:
         call lis_vector_duplicate(A,b,ierr)
27:
         call lis_vector_duplicate(A,x,ierr)
28:
         call lis_vector_set_all(1.0d0,u,ierr)
29:
         call lis_matvec(A,u,b,ierr)
30:
31:
         call lis_solver_create(solver,ierr)
32:
         call lis_solver_set_optionC(solver,ierr)
33:
         call lis_solve(A,b,x,solver,ierr)
34:
         call lis_solver_get_iter(solver,iter,ierr)
35:
         write(*,*) 'number of iterations = ',iter
36:
         call lis_vector_print(x,ierr)
37:
         call lis_matrix_destroy(A,ierr)
38:
         call lis_vector_destroy(b,ierr)
39:
         call lis_vector_destroy(x,ierr)
40:
         call lis_vector_destroy(u,ierr)
41:
         call lis_solver_destroy(solver,ierr)
42:
         call lis_finalize(ierr)
43:
44:
         stop
45:
         end
```

### 3.7 An Alternate Workflow: PSD

The previous section represents one of two workflows in Lis. The present workflow represents a decoupling of the preconditioner and the solver (Preconditioner and Solver Decoupled, or PSD), in the sense that the preconditioner can be updated separately from the solver; in the workflow presented in the previous section, the preconditioner is updated with every call to lis\_solve. This property (conditional updating of the preconditioner) turns out to be quite useful in solving certain problems, including some nonlinear partial differential equations. For nonlinear PDEs, iterative solution methods are used (e.g., Newton-Raphson) to calculate a solution. In the current context, each Newton-Raphson iteration calculates an incremental improvement to a solution vector via the solution of a linear system of equations. To support this functionality, the following (additional) functions must be used:

- lis\_matrix\_psd\_set\_value: Re-define the value of an existing matrix component.
- lis\_matrix\_psd\_reset\_scale: Set the matrix "scaled" status to *false*. Note that this call and the following one are only needed for the case non-trivial scaling.
- lis\_vector\_psd\_reset\_scale: Set the vector "scaled" status to false.
- lis\_solver\_set\_matrix: Associate the given matrix and solver. Note that this must be done before the call to lis\_precon\_psd\_create.
- lis\_precon\_psd\_create: Create data structures associated with the chosen preconditioner.
- lis\_precon\_psd\_update: Evaluate the preconditioner.

It is noted that this workflow currently has the following restrictions:

- The only matrix format currently supported is CSR.
- The only solver currently supported is GMRES.
- The only preconditioners currently supported are ILU(k) and SA-AMG.

Error checking has been implemented to prevent any unsupported cases from running.

The following pseudo-code listing presents an example of the workflow. An actual implementation can be seen in test problem test8f.F90.

```
- Pseudo-code example of workflow -
        PROGRAM psd_driver
 2:
 3:
        implicit none
 5:#include "lisf.h"
       LIS_INTEGER i,n,gn,is,ie,iter,ierr
 7:
 8:
       LIS_MATRIX A
 9:
       LIS_VECTOR b,x
10:
       LIS_SOLVER solver
11:
        REAL :: u(:),du
12:
13:
        CALL lis_initialize(ierr)
14:
       15:
       ! initialization, only done once
16:
       17:
18:
       CALL lis_matrix_create(LIS_COMM_WORLD,A,ierr)
        CALL lis_matrix_set_size(A,0,n,ierr)
19:
20:
        CALL lis_matrix_get_size(A,n,gn,ierr)
21:
        CALL lis_matrix_get_range(A,is,ie,ierr)
22:
23:
        CALL UpdateLinearSystem(RHS,LHS)
24:
        DO i=is,ie-1
25:
        DO j=1,gn
26:
              IF (LHS(i,j) exists) THEN
27:
                   CALL lis_matrix_set_value(LIS_INS_VALUE,i,j,LHS(i,j),A,ierr)
28:
             END IF
29:
          END DO
30:
       END DO
31:
        CALL lis_matrix_set_type(A,LIS_MATRIX_CSR,ierr)
32:
        CALL lis_matrix_assemble(A,ierr)
33:
34:
        CALL lis_vector_duplicate(A,b,ierr)
35:
        CALL lis_vector_duplicate(A,x,ierr)
36:
        DO i=is,ie-1
37:
            CALL lis_vector_set_value(LIS_INS_VALUE,i,RHS(i),b,ierr)
38:
       END DO
39:
       u = u_{initial}
40:
41:
        CALL lis_solver_create(solver,ierr)
        WRITE(UNIT=options,FMT='(a)') "-p ilu -i gmres -print out -scale none"
42:
43:
       CALL lis_solver_set_option(TRIM(options),solver,ierr)
44:
45:
       !-----
46:
       ! everything up to this point is more or less identical to the standard workflow.
47:
       ! Now comes the preconditioner initialization, and the Newton-Raphson
48:
       ! iteration.
49:
       50:
       CALL lis_solver_set_matrix(A,solver,ierr)
51:
       CALL lis_precon_psd_create(solver,precon,ierr)
52:
       ! evaluate the preconditioner, at least once . . .
53:
       CALL lis_precon_psd_update(solver,precon,ierr)
54:
```

```
- Pseudo-code example of workflow (contd.) -
 55:
 56:
 57:
             IF (UpdateLHS) THEN
 58:
                 DO i=is,ie-1
59:
                     DO j=1,gn
                         IF (component (i,j) exists) THEN
 60:
                             CALL lis_matrix_psd_set_value(LIS_INS_VALUE,i,j,LHS(i,j),A,ierr)
 61:
 62:
                         END IF
 63:
                     END DO
 64:
                  END DO
 65:
                  CALL lis_matrix_psd_reset_scale(A,ierr)
 66:
             END IF
 67:
 68:
             ! update RHS every iteration
 69:
             DO i=is,ie-1
                 CALL lis_vector_set_value(LIS_INS_VALUE,i,RHS(i),b,ierr)
70:
71:
             END DO
72:
             CALL lis_vector_psd_reset_scale(A,ierr)
73:
74:
             IF (UpdateLHS) THEN
75:
                 CALL lis_precon_psd_update(solver,precon,ierr)
76:
77:
             CALL lis_solve_kernel(A,b,x,solver,precon,ierr)
78:
             CALL lis_solver_get_iter(solver,iter,ierr)
79:
             write(*,*) 'number of iterations = ',iter
80:
             CALL lis_vector_print(x,ierr)
81:
             ! update the solution
82:
83:
             DO i=is,ie-1
84:
                 CALL lis_vector_get_value(x,i,du,ierr)
85:
                 u(i)=u(i)-du
             END DO
86:
87:
88:
             CALL UpdateLinearSystem(RHS,LHS)
89:
90:
             IF (termination criteria satisfied) EXIT
91:
92:
         END DO
93:
94:
          CALL lis_matrix_destroy(A,ierr)
95:
96:
          CALL lis_vector_destroy(b,ierr)
97:
          CALL lis_vector_destroy(x,ierr)
98:
          CALL lis_vector_destroy(u,ierr)
99:
          CALL lis_solver_destroy(solver,ierr)
100:
101:
          CALL lis_finalize(ierr)
102:
103:
          END PROGRAM psd_driver
```

## 3.8 Compiling and Linking

Provided below is an example test4.c located in the directory lis-(\$VERSION)/test, compiled on the SGI Altix 3700 using the Intel C/C++ Compiler (icc). Since the library includes some Fortran 90 codes when the SA-AMG preconditioner is selected, a Fortran 90 compiler must be used for the linking. The preprocessor macro USE\_MPI must be defined for the multiprocessing environment. The preprocessor macros LONG\_LONG for C and LONG\_LONG for Fortran must be defined when using the 64bit integer.

```
For the serial environment

Compiling

> icc -c -I($INSTALLDIR)/include test4.c

Linking

> icc -o test4 test4.o -L($INSTALLDIR)/lib -llis

Linking (with SA-AMG)

> ifort -nofor_main -o test4 test4.o -L($INSTALLDIR)/lib -llis
```

```
For multithreaded environment

Compiling

> icc -c -openmp -I($INSTALLDIR)/include test4.c

Linking

> icc -openmp -o test4 test4.o -L($INSTALLDIR)/lib -llis

Linking (with SA-AMG)

> ifort -nofor_main -openmp -o test4 test4.o -L($INSTALLDIR)/lib -llis
```

```
Compiling

> icc -c -DUSE_MPI -I($INSTALLDIR)/include test4.c

Linking

> icc -o test4 test4.o -L($INSTALLDIR)/lib -llis -lmpi

Linking (with SA-AMG)

> ifort -nofor_main -o test4 test4.o -L($INSTALLDIR)/lib -llis -lmpi
```

```
Compiling

> icc -c -openmp -DUSE_MPI -I($INSTALLDIR)/include test4.c

Linking

> icc -openmp -o test4 test4.o -L($INSTALLDIR)/lib -llis -lmpi

Linking (with SA-AMG)

> ifort -nofor_main -openmp -o test4 test4.o -L($INSTALLDIR)/lib -llis -lmpi
```

Provided below is an example test4f.F located in the directory lis-(\$VERSION)/test, compiled on the SGI Altix 3700 using the Intel Fortran Compiler (ifort). Since compiler directives are used in the program, an appropriate compiler option should be specified to use the preprocessor. -fpp is the option for the Intel compiler.

```
For serial environment

Compiling

> ifort -c -fpp -I($INSTALLDIR)/include test4f.F

Linking

> ifort -o test4f test4f.o -L($INSTALLDIR)/lib -llis
```

```
- For multithreaded environment -
    Compiling
       > ifort -c -fpp -openmp -I($INSTALLDIR)/include test4f.F
 Linking
       > ifort -openmp -o test4f test4f.o -L($INSTALLDIR)/lib -llis
   - For multiprocessing environment -
    Compiling
       > ifort -c -fpp -DUSE_MPI -I($INSTALLDIR)/include test4f.F
 Linking
       > ifort -o test4f test4f.o -L($INSTALLDIR)/lib -llis -lmpi
   - For multithreaded and multiprocessing environments -
    Compiling
       > ifort -c -fpp -openmp -DUSE_MPI -I($INSTALLDIR)/include test4f.F
 Linking
       > ifort -openmp -o test4f test4f.o -L($INSTALLDIR)/lib -llis -lmpi
3.9
      Running
The test programs test4 and test4f in the directory lis-($VERSION)/test are run as follows:
For serial environment
      > ./test4 -i bicgstab
For multithreaded environment
      > env OMP_NUM_THREADS=2 ./test4 -i bicgstab
For multiprocessing environment
      > mpirun -np 2 ./test4 -i bicgstab
For multithreaded and multiprocessing environment
      > mpirun -np 2 env OMP_NUM_THREADS=2 ./test4 -i bicgstab
The solution will be returned:
initial vector x
                     : all components set to 0
                      : double
precision
linear solver
                      : BiCGSTAB
preconditioner
                      : none
convergence condition : ||b-Ax||_2 \le 1.0e-12 * ||b-Ax_0||_2
matrix storage format : CSR
linear solver status : normal end
    0 1.000000e+000
    1 1.000000e+000
    2 1.000000e+000
    3 1.000000e+000
    4 1.000000e+000
    5 1.000000e+000
```

6 1.000000e+000 7 1.000000e+000 8 1.000000e+000 9 1.000000e+000

10 1.000000e+000

11 1.000000e+000

## 3.10 Zero DOFs on a Process

For the case of multiple MPI processes, it is possible to specify  $global\_n = 0$  and  $local\_n \ge 0$ . This will allow one or more MPI processes to have zero DOFs. However, it is still the case that, for  $global\_n = 0$ , the summation of  $local\_n$  over all processes should be greater than zero.

# 4 Quadruple Precision Operations

Double precision operations sometimes require a large number of iterations because of the rounding error. Besides long double precision operations, Lis supports "double-double" precision operations, or quadruple precision operations by combining two double precision floating point numbers [48, 49]. To use the double-double precision with the same interface as the double precision operations, both the matrix and vectors are assumed to be double precision. Lis also supports the performance acceleration of the double-double precision operations with the SIMD instructions, such as Intel's Streaming SIMD Extensions (SSE)[54].

## 4.1 Using Quadruple Precision Operations

The test program test5.c solves a linear equation Ax = b, where A is a Toeplitz matrix

$$\begin{pmatrix} 2 & 1 & & & & \\ 0 & 2 & 1 & & & \\ \gamma & 0 & 2 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & \gamma & 0 & 2 & 1 \\ & & & \gamma & 0 & 2 \end{pmatrix}.$$

The right-hand vector is set such that the values of the elements of the solution x are 1. The value n is the size of matrix A. test5 with option  $\neg f$  is run:

### Double precision

```
By entering > ./test5 200 2.0 -f double the following results will be returned:
```

```
n = 200, gamma = 2.000000
```

```
initial vector x: all components set to 0
```

precision : double
linear solver : BiCG
preconditioner : none

convergence condition :  $||b-Ax||_2 \le 1.0e-12 * ||b-Ax_0||_2$ 

matrix storage format : CSR

linear solver status : normal end

```
BiCG: number of iterations = 1001 (double = 1001, quad = 0)
```

 BiCG: elapsed time
 = 2.044368e-02 sec.

 BiCG: preconditioner
 = 4.768372e-06 sec.

 BiCG: matrix creation
 = 4.768372e-06 sec.

 BiCG: linear solver
 = 2.043891e-02 sec.

 BiCG: relative residual
 = 8.917591e+01

#### Quadruple precision

By entering > ./test5 200 2.0 -f quad the following results will be returned:

```
n = 200, gamma = 2.000000
```

initial vector  $\mathbf{x}$  : all components set to 0

precision : quad linear solver : BiCG preconditioner : none

convergence condition : ||b-Ax||\_2 <= 1.0e-12 \* ||b-Ax\_0||\_2

matrix storage format : CSR

linear solver status : normal end

BiCG: number of iterations = 230 (double = 230, quad = 0)

BiCG: elapsed time = 2.267408e-02 sec. BiCG: preconditioner = 4.549026e-04 sec. BiCG: matrix creation = 5.006790e-06 sec. BiCG: linear solver = 2.221918e-02 sec.

BiCG: relative residual = 6.499145e-11

# 5 Matrix Storage Formats

This section describes the matrix storage formats supported by the library. Assume that the matrix row (column) number begins with 0 and that the number of nonzero elements of matrix A of size  $n \times n$  is nnz.

## 5.1 Compressed Sparse Row (CSR)

The CSR format uses three arrays ptr, index and value to store data.

- ullet value is a double precision array of length nnz, which stores the nonzero elements of matrix A along the row.
- index is an integer array of length nnz, which stores the column numbers of the nonzero elements stored in the array value.
- ptr is an integer array of length n+1, which stores the starting points of the rows of the arrays value and index.

#### 5.1.1 Creating Matrices (for Serial and Multithreaded Environments)

The diagram on the right in Figure 2 shows how matrix A in Figure 2 is stored in the CSR format. A program to create the matrix in the CSR format is as follows:

Figure 2: Data structure of CSR format (for serial and multithreaded environments).

```
- For serial and multithreaded environments
 1: LIS_INT n,nnz;
 2: LIS_INT *ptr,*index;
3: LIS_SCALAR *value;
 4: LIS_MATRIX A;
 5: n = 4; nnz = 8;
 6: ptr = (LIS_INT *)malloc( (n+1)*sizeof(LIS_INT) );
7: index = (LIS_INT *)malloc( nnz*sizeof(LIS_INT) );
8: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
9: lis_matrix_create(0,&A);
10: lis_matrix_set_size(A,0,n);
12: ptr[0] = 0; ptr[1] = 1; ptr[2] = 3; ptr[3] = 5; ptr[4] = 8;
13: index[0] = 0; index[1] = 0; index[2] = 1; index[3] = 1;
14: index[4] = 2; index[5] = 0; index[6] = 2; index[7] = 3;
15: value[0] = 11; value[1] = 21; value[2] = 22; value[3] = 32;
16: value[4] = 33; value[5] = 41; value[6] = 43; value[7] = 44;
18: lis_matrix_set_csr(nnz,ptr,index,value,A);
19: lis_matrix_assemble(A);
```

## 5.1.2 Creating Matrices (for Multiprocessing Environment)

Figure 3 shows how matrix A in Figure 2 is stored in the CSR format on two processing elements. A program to create the matrix in the CSR format on two processing elements is as follows:



Figure 3: Data structure of CSR format (for multiprocessing environment).

```
    For multiprocessing environment -

 1: LIS_INT i,k,n,nnz,my_rank;
2: LIS_INT *ptr,*index;
3: LIS_SCALAR *value;
 4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
6: if( my_rank==0 ) {n = 2; nnz = 3;}
7: else
                     {n = 2; nnz = 5;}
8: ptr = (LIS_INT *)malloc( (n+1)*sizeof(LIS_INT) );
9: index = (LIS_INT *)malloc( nnz*sizeof(LIS_INT) );
10: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
11: lis_matrix_create(MPI_COMM_WORLD,&A);
12: lis_matrix_set_size(A,n,0);
13: if( my_rank==0 ) {
14:
        ptr[0] = 0; ptr[1] = 1; ptr[2] = 3;
15:
        index[0] = 0; index[1] = 0; index[2] = 1;
        value[0] = 11; value[1] = 21; value[2] = 22;}
16:
17: else {
        ptr[0] = 0; ptr[1] = 2; ptr[2] = 5;
18:
19:
        index[0] = 1; index[1] = 2; index[2] = 0; index[3] = 2; index[4] = 3;
        value[0] = 32; value[1] = 33; value[2] = 41; value[3] = 43; value[4] = 44;}
21: lis_matrix_set_csr(nnz,ptr,index,value,A);
22: lis_matrix_assemble(A);
```

#### 5.1.3 Associating Arrays

To associate the arrays in the CSR format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_csr(LIS\_INT nnz, LIS\_INT ptr[], LIS\_INT index[], LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_csr(LIS\_INTEGER nnz, LIS\_INTEGER ptr(), LIS\_INTEGER index(), LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

# 5.2 Compressed Sparse Column (CSC)

The CSS format uses three arrays ptr, index and value to store data.

- value is a double precision array of length nnz, which stores the nonzero elements of matrix A along the column.
- index is an integer array of length nnz, which stores the row numbers of the nonzero elements stored in the array value.
- ptr is an integer array of length n + 1, which stores the starting points of the rows of the arrays value and index.

### 5.2.1 Creating Matrices (for Serial and Multithreaded Environments)

The diagram on the right in Figure 4 shows how matrix A in Figure 4 is stored in the CSC format. A program to create the matrix in the CSC format is as follows:

Figure 4: Data structure of CSC format (for serial and multithreaded environments).

```
- For serial and multithreaded environments -
 1: LIS_INT n,nnz;
 2: LIS_INT *ptr,*index;
3: LIS_SCALAR *value;
 4: LIS_MATRIX A;
5: n = 4; nnz = 8;
 6: ptr = (LIS_INT *)malloc( (n+1)*sizeof(LIS_INT) );
7: index = (LIS_INT *)malloc( nnz*sizeof(LIS_INT) );
8: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
9: lis_matrix_create(0,&A);
10: lis_matrix_set_size(A,0,n);
11:
12: ptr[0] = 0; ptr[1] = 3; ptr[2] = 5; ptr[3] = 7; ptr[4] = 8;
13: index[0] = 0; index[1] = 1; index[2] = 3; index[3] = 1;
14: index[4] = 2; index[5] = 2; index[6] = 3; index[7] = 3;
15: value[0] = 11; value[1] = 21; value[2] = 41; value[3] = 22;
16: value[4] = 32; value[5] = 33; value[6] = 43; value[7] = 44;
18: lis_matrix_set_csc(nnz,ptr,index,value,A);
19: lis_matrix_assemble(A);
```

## 5.2.2 Creating Matrices (for Multiprocessing Environment)

Figure 5 shows how matrix A in Figure 4 is stored on two processing elements. A program to create the matrix in the CSC format on two processing elements is as follows:



Figure 5: Data structure of CSC format (for multiprocessing environment).

```
- For multiprocessing environment -
 1: LIS_INT i,k,n,nnz,my_rank;
2: LIS_INT *ptr,*index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
6: if( my_rank==0 ) {n = 2; nnz = 3;}
7: else
                     {n = 2; nnz = 5;}
8: ptr = (LIS_INT *)malloc( (n+1)*sizeof(LIS_INT) );
9: index = (LIS_INT *)malloc( nnz*sizeof(LIS_INT) );
10: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
11: lis_matrix_create(MPI_COMM_WORLD,&A);
12: lis_matrix_set_size(A,n,0);
13: if( my_rank==0 ) {
14:
        ptr[0] = 0; ptr[1] = 3; ptr[2] = 5;
        index[0] = 0; index[1] = 1; index[2] = 3; index[3] = 1; index[4] = 2;
15:
        value[0] = 11; value[1] = 21; value[2] = 41; value[3] = 22; value[4] = 32}
16:
17: else {
        ptr[0] = 0; ptr[1] = 2; ptr[2] = 3;
18:
19:
        index[0] = 2; index[1] = 3; index[2] = 3;
        value[0] = 33; value[1] = 43; value[2] = 44;}
21: lis_matrix_set_csc(nnz,ptr,index,value,A);
22: lis_matrix_assemble(A);
```

#### 5.2.3 Associating Arrays

To associate the arrays in the CSC format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_csc(LIS\_INT nnz, LIS\_INT row[], LIS\_INT index[], LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_csc(LIS\_INTEGER nnz, LIS\_INTEGER row(), LIS\_INTEGER index(), LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

## 5.3 Modified Compressed Sparse Row (MSR)

The MSR format uses two arrays index and value to store data. Assume that ndz represents the number of zero elements of the diagonal.

- value is a double precision array of length nnz + ndz + 1, which stores the diagonal of matrix A down to the n-th element. The n + 1-th element is not used. For the n + 2-th and after, the values of the nonzero elements except the diagonal of matrix A are stored along the row.
- index is an integer array of length nnz + ndz + 1, which stores the starting points of the rows of the off-diagonal elements of matrix A down to the n + 1-th element. For the n + 2-th and after, it stores the row numbers of the off-diagonal elements of matrix A stored in the array value.

### 5.3.1 Creating Matrices (for Serial and Multithreaded Environments)

The diagram on the right in Figure 6 shows how matrix A is stored in the MSR format. A program to create the matrix in the MSR format is as follows:

Figure 6: Data structure of MSR format (for serial and multithreaded environments).

```
    For serial and multithreaded environments -

 1: LIS_INT n,nnz,ndz;
 2: LIS_INT *index;
3: LIS_SCALAR *value;
 4: LIS_MATRIX A;
5: n = 4; nnz = 8; ndz = 0;
 6: index = (LIS_INT *)malloc( (nnz+ndz+1)*sizeof(LIS_INT) );
7: value = (LIS_SCALAR *)malloc( (nnz+ndz+1)*sizeof(LIS_SCALAR) );
8: lis_matrix_create(0,&A);
9: lis_matrix_set_size(A,0,n);
11: index[0] = 5; index[1] = 5; index[2] = 6; index[3] = 7;
12: index[4] = 9; index[5] = 0; index[6] = 1; index[7] = 0; index[8] = 2;
13: value[0] = 11; value[1] = 22; value[2] = 33; value[3] = 44;
14: value[4] = 0; value[5] = 21; value[6] = 32; value[7] = 41; value[8] = 43;
16: lis_matrix_set_msr(nnz,ndz,index,value,A);
17: lis_matrix_assemble(A);
```

## 5.3.2 Creating Matrices (for Multiprocessing Environment)

Figure 7 shows how matrix A in Figure 6 is stored in the MSR format on two processing elements. A program to create the matrix in the MSR format on two processing element is as follows:



Figure 7: Data structure of MSR format (for multiprocessing environment).

```
- For multiprocessing environment -
 1: LIS_INT i,k,n,nnz,ndz,my_rank;
2: LIS_INT *index;
3: LIS_SCALAR *value;
 4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
 6: if( my_rank==0 ) {n = 2; nnz = 3; ndz = 0;}
                     {n = 2; nnz = 5; ndz = 0;}
7: else
8: index = (LIS_INT *)malloc( (nnz+ndz+1)*sizeof(LIS_INT) );
9: value = (LIS_SCALAR *)malloc( (nnz+ndz+1)*sizeof(LIS_SCALAR) );
10: lis_matrix_create(MPI_COMM_WORLD,&A);
11: lis_matrix_set_size(A,n,0);
12: if( my_rank==0 ) {
        index[0] = 3; index[1] = 3; index[2] = 4; index[3] = 0;
13:
        value[0] = 11; value[1] = 22; value[2] = 0; value[3] = 21;}
14:
15: else {
        index[0] = 3; index[1] = 4; index[2] = 6; index[3] = 1;
16:
        index[4] = 0; index[5] = 2;
17:
        value[0] = 33; value[1] = 44; value[2] = 0; value[3] = 32;
18:
19:
        value[4] = 41; value[5] = 43;}
20: lis_matrix_set_msr(nnz,ndz,index,value,A);
21: lis_matrix_assemble(A);
```

#### 5.3.3 Associating Arrays

To associate the arrays in the MSR format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_msr(LIS\_INT nnz, LIS\_INT ndz, LIS\_INT index[], LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_msr(LIS\_INTEGER nnz, LIS\_INTEGER ndz, LIS\_INTEGER index(), LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

## Diagonal (DIA)

The DIA format uses two arrays index and value to store data. Assume that nnd represents the number of nonzero diagonal elements of matrix A.

- value is a double precision array of length  $nnd \times n$ , which stores the values of the nonzero diagonal elements of matrix A.
- index is an integer array of length nnd, which stores the offsets from the main diagonal.

For the multithreaded environment, the following modifications have been made: the format uses two arrays index and value to store data. Assume that nprocs represents the number of threads.  $nnd_n$  is the number of nonzero diagonal elements of the partial matrix into which the row block of matrix A is divided. maxnnd is the maximum value  $nnd_p$ .

- value is a double precision array of length  $maxnnd \times n$ , which stores the values of the nonzero diagonal elements of matrix A.
- index is an integer array of length nprocs × maxnnd, which stores the offsets from the main diagonal.

#### 5.4.1 Creating Matrices (for Serial Environment)

The diagram on the right in Figure 8 shows how matrix A in Figure 8 is stored in the DIA format. A program to create the matrix in the DIA format is as follows:

$$A = \begin{pmatrix} 11 & & & \\ 21 & 22 & & & \\ & 32 & 33 & \\ 41 & & 43 & 44 \end{pmatrix} \begin{bmatrix} -3 & -1 & 0 & & \\ \hline 0 & 0 & 041 & 021 & 32 & 43 & 11 & 22 & 33 & 44 \end{bmatrix}$$
 A.index A.value

Figure 8: Data structure of DIA format (for serial environment).

```
- For serial environment -
 1: LIS_INT n,nnd;
 2: LIS_INT *index;
 3: LIS_SCALAR *value;
 4: LIS_MATRIX A;
5: n = 4; nnd = 3;
 6: index = (LIS_INT *)malloc( nnd*sizeof(LIS_INT) );
7: value = (LIS_SCALAR *)malloc( n*nnd*sizeof(LIS_SCALAR) );
8: lis_matrix_create(0,&A);
9: lis_matrix_set_size(A,0,n);
10:
11: index[0] = -3; index[1] = -1; index[2] = 0;
12: value[0] = 0; value[1] = 0; value[2] = 0; value[3] = 41;
13: value[4] = 0; value[5] = 21; value[6] = 32; value[7] = 43;
14: value[8] = 11; value[9] = 22; value[10] = 33; value[11] = 44;
15:
16: lis_matrix_set_dia(nnd,index,value,A);
17: lis_matrix_assemble(A);
```

## 5.4.2 Creating Matrices (for Multithreaded Environment)

Figure 9 shows how matrix A in Figure 8 is stored in the DIA format on two threads. A program to create the matrix in the DIA format on two threads is as follows:

-1	0		-3	-1	0							A.index
0	21	11	22			0	41	32	43	33	44	A.value

Figure 9: Data structure of DIA format (for multithreaded environment).

```
- For multithreaded environment -
 1: LIS_INT n,maxnnd,nprocs;
2: LIS_INT *index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 4; maxnnd = 3; nprocs = 2;
6: index = (LIS_INT *)malloc( maxnnd*sizeof(LIS_INT) );
7: value = (LIS_SCALAR *)malloc( n*maxnnd*sizeof(LIS_SCALAR) );
8: lis_matrix_create(0,&A);
9: lis_matrix_set_size(A,0,n);
10:
11: index[0] = -1; index[1] = 0; index[2] = 0; index[3] = -3; index[4] = -1; index[5] = 0;
12: value[0] = 0; value[1] = 21; value[2] = 11; value[3] = 22; value[4] = 0; value[5] = 0;
13: value[6] = 0; value[7] = 41; value[8] = 32; value[9] = 43; value[10] = 33; value[11] = 44;
15: lis_matrix_set_dia(maxnnd,index,value,A);
16: lis_matrix_assemble(A);
```

## 5.4.3 Creating Matrices (for Multiprocessing Environment)

Figure 10 shows how matrix A in Figure 8 is stored in the DIA format on two processing elements. A program to create the matrix in the DIA format on two processing elements is as follows:



Figure 10: Data structure of DIA format (for multiprocessing environment).

```
    For multiprocessing environment ——

 1: LIS_INT i,n,nnd,my_rank;
2: LIS_INT *index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
 6: if( my_rank==0 ) {n = 2; nnd = 2;}
7: else
                     {n = 2; nnd = 3;}
8: index = (LIS_INT *)malloc( nnd*sizeof(LIS_INT) );
9: value = (LIS_SCALAR *)malloc( n*nnd*sizeof(LIS_SCALAR) );
10: lis_matrix_create(MPI_COMM_WORLD,&A);
11: lis_matrix_set_size(A,n,0);
12: if( my_rank==0 ) {
13:
        index[0] = -1; index[1] = 0;
        value[0] = 0; value[1] = 21; value[2] = 11; value[3] = 22;}
14:
15: else {
16:
        index[0] = -3; index[1] = -1; index[2] = 0;
        value[0] = 0; value[1] = 41; value[2] = 32; value[3] = 43; value[4] = 33;
17:
        value[5] = 44;
18:
19: lis_matrix_set_dia(nnd,index,value,A);
20: lis_matrix_assemble(A);
```

### 5.4.4 Associating Arrays

To associate the arrays in the DIA format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_dia(LIS\_INT nnd, LIS\_INT index[], LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_dia(LIS\_INTEGER nnd, LIS\_INTEGER index(), LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

### 5.5 Ellpack-Itpack Generalized Diagonal (ELL)

The ELL format uses two arrays index and value to store data. Assume that maxnzr is the maximum value of the number of nonzero elements in the rows of matrix A.

- value is a double precision array of length  $maxnzr \times n$ , which stores the values of the nonzero elements of the rows of matrix A along the column. The first column consists of the first nonzero elements of each row. If there is no nonzero elements to be stored, then 0 is stored.
- index is an integer array of length  $maxnzr \times n$ , which stores the column numbers of the nonzero elements stored in the array value. If the number of nonzero elements in the *i*-th row is nnz, then index  $[nnz \times n + i]$  stores row number *i*.

### 5.5.1 Creating Matrices (for Serial and Multithreaded Environments)

The diagram on the right in Figure 11 shows how matrix A in Figure 11 is stored in the ELL format. A program to create the matrix in the ELL format is as follows:

Figure 11: Data structure of ELL format (for serial and multithreaded environments).

```
- For serial and multithreaded environments -
 1: LIS_INT n,maxnzr;
 2: LIS_INT *index;
3: LIS_SCALAR *value;
 4: LIS_MATRIX A;
 5: n = 4; maxnzr = 3;
 6: index = (LIS_INT *)malloc( n*maxnzr*sizeof(LIS_INT) );
7: value = (LIS_SCALAR *)malloc( n*maxnzr*sizeof(LIS_SCALAR) );
8: lis_matrix_create(0,&A);
9: lis_matrix_set_size(A,0,n);
11: index[0] = 0; index[1] = 0; index[2] = 1; index[3] = 0; index[4] = 0; index[5] = 1;
12: index[6] = 2; index[7] = 2; index[8] = 0; index[9] = 1; index[10] = 2; index[11] = 3;
13: value[0] = 11; value[1] = 21; value[2] = 32; value[3] = 41; value[4] = 0; value[5] = 22;
14: value[6] = 33; value[7] = 43; value[8] = 0; value[9] = 0; value[10] = 0; value[11] = 44;
16: lis_matrix_set_ell(maxnzr,index,value,A);
17: lis_matrix_assemble(A);
```

## 5.5.2 Creating Matrices (for Multiprocessing Environment)

Figure 12 shows how matrix A in Figure 11 is stored in the ELL format. A program to create the matrix in the ELL format on two processing elements is as follows:

0 0 0 1	1 0 2 2 3	A.inde
11 21 0 22	32 41 33 43 0 44	A.valu
PE0	PE1	

Figure 12: Data structure of ELL format (for multiprocessing environment).

```
    For multiprocessing environment —

 1: LIS_INT i,n,maxnzr,my_rank;
2: LIS_INT *index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
 6: if( my_rank==0 ) {n = 2; maxnzr = 2;}
7: else
                     {n = 2; maxnzr = 3;}
8: index = (LIS_INT *)malloc( n*maxnzr*sizeof(LIS_INT) );
9: value = (LIS_SCALAR *)malloc( n*maxnzr*sizeof(LIS_SCALAR) );
10: lis_matrix_create(MPI_COMM_WORLD,&A);
11: lis_matrix_set_size(A,n,0);
12: if( my_rank==0 ) {
13:
        index[0] = 0; index[1] = 0; index[2] = 0; index[3] = 1;
        value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;}
14:
15: else {
16:
        index[0] = 1; index[1] = 0; index[2] = 2; index[3] = 2; index[4] = 2;
        index[5] = 3;
17:
        value[0] = 32; value[1] = 41; value[2] = 33; value[3] = 43; value[4] = 0;
18:
        value[5] = 44;
19:
20: lis_matrix_set_ell(maxnzr,index,value,A);
21: lis_matrix_assemble(A);
```

#### 5.5.3 Associating Arrays

To associate an array required by the ELL format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_ell(LIS\_INT maxnzr, LIS\_INT index[], LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_ell(LIS\_INTEGER maxnzr, LIS\_INTEGER index(), LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

## 5.6 Jagged Diagonal (JAD)

The JAD format first sorts the nonzero elements of the rows in decreasing order of size, and then stores them along the column. The JAD format uses four arrays, perm, ptr, index, and value, to store data. Assume that maxnzr represents the maximum value of the number of nonzero elements of matrix A.

- $\bullet$  perm is an integer array of length n, which stores the sorted row numbers.
- value is a double precision array of length nnz, which stores the values of the jagged diagonal elements of the sorted matrix A. The first jagged diagonal consists of the values of the first nonzero elements of each row. The next jagged diagonal consists of the values of the second nonzero elements, and so on.
- index is an integer array of length nnz, which stores the row numbers of the nonzero elements stored in the array value.
- ptr is an integer array of length maxnzr+1, which stores the starting points of the jagged diagonal elements.

For the multithreaded environment, the following modifications have been made: the format uses four arrays, perm, ptr, index, and value, to store data. Assume that nprocs is the number of threads.  $maxnzr_p$  is the number of nonzero diagonal elements of the partial matrix into which the row block of matrix A is divided. maxmaxnzr is the maximum value of  $maxnzr_p$ .

- perm is an integer array of length n, which stores the sorted row numbers.
- value is a double precision array of length nnz, which stores the values of the jagged diagonal elements of the sorted matrix A. The first jagged diagonal consists of the values of the first nonzero elements of each row. The next jagged diagonal consist of the values of the second nonzero elements of each row, and so on.
- index is an integer array of length nnz, which stores the row numbers of the nonzero elements stored in the array value.
- ptr is an integer array of length  $nprocs \times (maxmaxnzr + 1)$ , which stores the starting points of the jagged diagonal elements.

## 5.6.1 Creating Matrices (for Serial Environment)

The diagram on the right in Figure 13 shows how matrix A in Figure 13 is stored in the JAD format. A program to create the matrix in the JAD format is as follows:



Figure 13: Data structure of JAD format (for serial environment).

```
- For serial environment -
 1: LIS_INT n,nnz,maxnzr;
 2: LIS_INT *perm,*ptr,*index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 4; nnz = 8; maxnzr = 3;
 6: perm = (LIS_INT *)malloc( n*sizeof(LIS_INT) );
7: ptr = (LIS_INT *)malloc( (maxnzr+1)*sizeof(LIS_INT) );
8: index = (LIS_INT *)malloc( nnz*sizeof(LIS_INT) );
9: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
10: lis_matrix_create(0,&A);
11: lis_matrix_set_size(A,0,n);
12:
13: perm[0] = 3; perm[1] = 1; perm[2] = 2; perm[3] = 0;
14: ptr[0] = 0; ptr[1] = 4; ptr[2] = 7; ptr[3] = 8;
15: index[0] = 0; index[1] = 0; index[2] = 1; index[3] = 0;
16: index[4] = 2; index[5] = 1; index[6] = 2; index[7] = 3;
17: value[0] = 41; value[1] = 21; value[2] = 32; value[3] = 11;
18: value[4] = 43; value[5] = 22; value[6] = 33; value[7] = 44;
20: lis_matrix_set_jad(nnz,maxnzr,perm,ptr,index,value,A);
21: lis_matrix_assemble(A);
```

## 5.6.2 Creating Matrices (for Multithreaded Environment)

Figure 14 shows how matrix A in Figure 13 is stored in the JAD format on two threads. A program to create the matrix in the JAD format on two threads is as follows:



Figure 14: Data structure of JAD format (for multithreaded environment).

```
- For multithreaded environment -
 1: LIS_INT n,nnz,maxmaxnzr,nprocs;
 2: LIS_INT *perm,*ptr,*index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 4; nnz = 8; maxmaxnzr = 3; nprocs = 2;
 6: perm = (LIS_INT *)malloc( n*sizeof(LIS_INT) );
7: ptr = (LIS_INT *)malloc( nprocs*(maxmaxnzr+1)*sizeof(LIS_INT) );
8: index = (LIS_INT *)malloc( nnz*sizeof(LIS_INT) );
9: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
10: lis_matrix_create(0,&A);
11: lis_matrix_set_size(A,0,n);
13: perm[0] = 1; perm[1] = 0; perm[2] = 3; perm[3] = 2;
14: ptr[0] = 0; ptr[1] = 2; ptr[2] = 3; ptr[3] = 0;
15: ptr[4] = 3; ptr[5] = 5; ptr[6] = 7; ptr[7] = 8;
16: index[0] = 0; index[1] = 0; index[2] = 1; index[3] = 0;
17: index[4] = 1; index[5] = 2; index[6] = 2; index[7] = 3;
18: value[0] = 21; value[1] = 11; value[2] = 22; value[3] = 41;
19: value[4] = 32; value[5] = 43; value[6] = 33; value[7] = 44;
20:
21: lis_matrix_set_jad(nnz,maxmaxnzr,perm,ptr,index,value,A);
22: lis_matrix_assemble(A);
```

## 5.6.3 Creating Matrices (for Multiprocessing Environment)

Figure 15 shows how matrix A in Figure 13 is stored in the JAD format on two processing elements. A program to create the matrix in the JAD format on two processing elements is as follows:



Figure 15: Data structure of JAD format (for multiprocessing environment).

```
- For multiprocessing environment -
 1: LIS_INT i,n,nnz,maxnzr,my_rank;
 2: LIS_INT *perm,*ptr,*index;
3: LIS_SCALAR *value;
 4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
 6: if( my_rank==0 ) {n = 2; nnz = 3; maxnzr = 2;}
                     {n = 2; nnz = 5; maxnzr = 3;}
8: perm = (LIS_INT *)malloc( n*sizeof(LIS_INT) );
9: ptr = (LIS_INT *)malloc( (maxnzr+1)*sizeof(LIS_INT) );
10: index = (LIS_INT *)malloc( nnz*sizeof(LIS_INT) );
11: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
12: lis_matrix_create(MPI_COMM_WORLD,&A);
13: lis_matrix_set_size(A,n,0);
14: if( my_rank==0 ) {
15:
        perm[0] = 1; perm[1] = 0;
16:
        ptr[0] = 0; ptr[1] = 2; ptr[2] = 3;
        index[0] = 0; index[1] = 0; index[2] = 1;
17:
18:
        value[0] = 21; value[1] = 11; value[2] = 22;}
19: else {
20:
        perm[0] = 3; perm[1] = 2;
        ptr[0] = 0; ptr[1] = 2; ptr[2] = 4; ptr[3] = 5;
21:
        index[0] = 0; index[1] = 1; index[2] = 2; index[3] = 2; index[4] = 3;
22:
        value[0] = 41; value[1] = 32; value[2] = 43; value[3] = 33; value[4] = 44;}
24: lis_matrix_set_jad(nnz,maxnzr,perm,ptr,index,value,A);
25: lis_matrix_assemble(A);
```

### 5.6.4 Associating Arrays

To associate an array required by the JAD format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_jad(LIS\_INT nnz, LIS\_INT maxnzr, LIS\_INT perm[], LIS\_INT ptr[], LIS\_INT index[], LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_jad(LIS\_INTEGER nnz, LIS\_INTEGER maxnzr, LIS\_INTEGER perm(), LIS\_INTEGER ptr(), LIS\_INTEGER index(), LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

## 5.7 Block Sparse Row (BSR)

The BSR format breaks down matrix A into partial matrices called blocks of size  $r \times c$ . The BSR format stores the nonzero blocks, in which at least one nonzero element exists, in a format similar to that of CSR. Assume that nr = n/r and bnnz are the numbers of nonzero blocks of A. The BSR format uses three arrays bptr, bindex and value to store data.

- value is a double precision array of length  $bnnz \times r \times c$ , which stores the values of the elements of the nonzero blocks.
- $\bullet$  bindex is an integer array of length bnnz, which stores the block column numbers of the nonzero blocks.
- bptr is an integer array of length nr + 1, which stores the starting points of the block rows in the array bindex.

#### 5.7.1 Creating Matrices (for Serial and Multithreaded Environments)

The diagram on the right in Figure 16 shows how matrix A in Figure 16 is stored in the BSR format. A program to create the matrix in the BSR format is as follows:

$$A = \begin{pmatrix} 11 & & & & & \\ 21 & 22 & & & & \\ \hline & 32 & 33 & & \\ 41 & & 43 & 44 \end{pmatrix} \begin{pmatrix} 0 & 1 & 3 & & & \\ \hline & 0 & 0 & 1 & & & \\ \hline & 0 & 0 & 1 & & & \\ \hline & 11 & 21 & 0 & 22 & 0 & 41 & 32 & 0 & 33 & 43 & 0 & 44 & \\ \hline & A. \text{ bindex} \\ & A. \text{value} \end{pmatrix}$$

Figure 16: Data structure of BSR format (for serial and multithreaded environments).

```
- For serial and multithreaded environments
 1: LIS_INT n,bnr,bnc,nr,nc,bnnz;
 2: LIS_INT *bptr,*bindex;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 4; bnr = 2; bnc = 2; bnnz = 3; nr = (n-1)/bnr+1; nc = (n-1)/bnc+1;
          = (LIS_INT *)malloc( (nr+1)*sizeof(LIS_INT) );
 7: bindex = (LIS_INT *)malloc( bnnz*sizeof(LIS_INT) );
8: value = (LIS_SCALAR *)malloc( bnr*bnc*bnnz*sizeof(LIS_SCALAR) );
9: lis_matrix_create(0,&A);
10: lis_matrix_set_size(A,0,n);
11:
12: bptr[0] = 0; bptr[1] = 1; bptr[2] = 3;
13: bindex[0] = 0; bindex[1] = 0; bindex[2] = 1;
14: value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;
15: value[4] = 0; value[5] = 41; value[6] = 32; value[7] = 0;
16: value[8] = 33; value[9] = 43; value[10] = 0; value[11] = 44;
18: lis_matrix_set_bsr(bnr,bnc,bnnz,bptr,bindex,value,A);
19: lis_matrix_assemble(A);
```

## 5.7.2 Creating Matrices (for Multiprocessing Environment)

Figure 17 shows how matrix A in Figure 16 is stored in the BSR format on two processing elements. A program to create the matrix in the BSR format on two processing elements is as follows:



Figure 17: Data structure of BSR format (for multiprocessing environment).

```
    For multiprocessing environment -

 1: LIS_INT n,bnr,bnc,nr,nc,bnnz,my_rank;
2: LIS_INT *bptr,*bindex;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
 6: if( my_rank==0 ) {n = 2; bnr = 2; bnc = 2; bnnz = 1; nr = (n-1)/bnr+1; nc = (n-1)/bnc+1;}
                     {n = 2; bnr = 2; bnc = 2; bnnz = 2; nr = (n-1)/bnr+1; nc = (n-1)/bnc+1;}
           = (LIS_INT *)malloc( (nr+1)*sizeof(LIS_INT) );
9: bindex = (LIS_INT *)malloc( bnnz*sizeof(LIS_INT) );
10: value = (LIS_SCALAR *)malloc( bnr*bnc*bnnz*sizeof(LIS_SCALAR) );
11: lis_matrix_create(MPI_COMM_WORLD,&A);
12: lis_matrix_set_size(A,n,0);
13: if( my_rank==0 ) {
14:
        bptr[0] = 0; bptr[1] = 1;
15:
        bindex[0] = 0;
        value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;}
16:
17: else {
18:
        bptr[0] = 0; bptr[1] = 2;
19:
        bindex[0] = 0; bindex[1] = 1;
        value[0] = 0; value[1] = 41; value[2] = 32; value[3] = 0;
20:
        value[4] = 33; value[5] = 43; value[6] = 0; value[7] = 44;}
21:
22: lis_matrix_set_bsr(bnr,bnc,bnnz,bptr,bindex,value,A);
23: lis_matrix_assemble(A);
```

### 5.7.3 Associating Arrays

To associate the arrays in the BSR format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_bsr(LIS\_INT bnr, LIS\_INT bnc, LIS\_INT bnnz, LIS\_INT bptr[], LIS\_INT bindex[], LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_bsr(LIS\_INTEGER bnr, LIS\_INTEGER bnc, LIS\_INTEGER bnnz, LIS\_INTEGER bptr(), LIS\_INTEGER bindex(), LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

## 5.8 Block Sparse Column (BSC)

The BSC format breaks down matrix A into partial matrices called blocks of size  $r \times c$ . The BSC format stores the nonzero blocks, in which at least one nonzero element exists, in a format similar to that of CSC. Assume that nc = n/c and bnnz are the numbers of the nonzero blocks of A. The BSC format uses three arrays bptr, bindex and value to store data.

- value is a double precision array of length  $bnnz \times r \times c$ , which stores the values of the elements of the nonzero blocks.
- bindex is an integer array of length bnnz, which stores the block row numbers of the nonzero blocks.
- bptr is an integer array of length nc + 1, which stores the starting points of the block columns in the array bindex.

### 5.8.1 Creating Matrices (for Serial and Multithreaded Environments)

The diagram on the right in Figure 18 shows how matrix A in Figure 18 is stored in the BSC format. A program to create the matrix in the BSC format is as follows:

$$A = \begin{pmatrix} 11 & & & & \\ 21 & 22 & & & \\ \hline & 32 & 33 & \\ 41 & & 43 & 44 \end{pmatrix} \begin{pmatrix} \textbf{0} & \textbf{1} & \textbf{3} & & \\ \textbf{0} & \textbf{1} & \textbf{1} & & \\ \hline & \textbf{0} & \textbf{1} & \textbf{21} & \textbf{0} & \textbf{22} & \textbf{0} & \textbf{41} & \textbf{32} & \textbf{0} & \textbf{33} & \textbf{43} & \textbf{0} & \textbf{44} \\ \hline & \textbf{11} & \textbf{21} & \textbf{0} & \textbf{22} & \textbf{0} & \textbf{41} & \textbf{32} & \textbf{0} & \textbf{33} & \textbf{43} & \textbf{0} & \textbf{44} \\ \hline \end{pmatrix} & \textbf{A.bindex}$$

Figure 18: Data structure of BSC format (for serial and multithreaded environments).

```
- For serial and multithreaded environments -
 1: LIS_INT n,bnr,bnc,nr,nc,bnnz;
 2: LIS_INT *bptr,*bindex;
 3: LIS_SCALAR *value;
 4: LIS_MATRIX A;
5: n = 4; bnr = 2; bnc = 2; bnnz = 3; nr = (n-1)/bnr+1; nc = (n-1)/bnc+1;
         = (LIS_INT *)malloc( (nc+1)*sizeof(LIS_INT) );
7: bindex = (LIS_INT *)malloc( bnnz*sizeof(LIS_INT) );
8: value = (LIS_SCALAR *)malloc( bnr*bnc*bnnz*sizeof(LIS_SCALAR) );
9: lis_matrix_create(0,&A);
10: lis_matrix_set_size(A,0,n);
11:
12: bptr[0] = 0; bptr[1] = 1; bptr[2] = 3;
13: bindex[0] = 0; bindex[1] = 1; bindex[2] = 1;
14: value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;
15: value[4] = 0; value[5] = 41; value[6] = 32; value[7] = 0;
16: value[8] = 33; value[9] = 43; value[10] = 0; value[11] = 44;
17:
18: lis_matrix_set_bsc(bnr,bnc,bnnz,bptr,bindex,value,A);
19: lis_matrix_assemble(A);
```

## 5.8.2 Creating Matrices (for Multiprocessing Environment)

Figure 19 shows how matrix A in Figure 18 is stored in the BSC format on two processing elements. A program to create the matrix in the BSC format on two processing elements is as follows:



Figure 19: Data structure of BSC format (for multiprocessing environment).

```
    For multiprocessing environment -

 1: LIS_INT n,bnr,bnc,nr,nc,bnnz,my_rank;
2: LIS_INT *bptr,*bindex;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
 6: if( my_n = 0 ) {n = 2; bnr = 2; bnc = 2; bnnz = 2; nr = (n-1)/bnr + 1; nc = (n-1)/bnc + 1;}
                     {n = 2; bnr = 2; bnc = 2; bnnz = 1; nr = (n-1)/bnr+1; nc = (n-1)/bnc+1;}
           = (LIS_INT *)malloc( (nr+1)*sizeof(LIS_INT) );
9: bindex = (LIS_INT *)malloc( bnnz*sizeof(LIS_INT) );
10: value = (LIS_SCALAR *)malloc( bnr*bnc*bnnz*sizeof(LIS_SCALAR) );
11: lis_matrix_create(MPI_COMM_WORLD,&A);
12: lis_matrix_set_size(A,n,0);
13: if( my_rank==0 ) {
        bptr[0] = 0; bptr[1] = 2;
14:
15:
        bindex[0] = 0; bindex[1] = 1;
        value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;
16:
        value[4] = 0; value[5] = 41; value[6] = 32; value[7] = 0;}
17:
18: else {
19:
        bptr[0] = 0; bptr[1] = 1;
20:
        bindex[0] = 1;
        value[0] = 33; value[1] = 43; value[2] = 0; value[3] = 44;}
21:
22: lis_matrix_set_bsc(bnr,bnc,bnnz,bptr,bindex,value,A);
23: lis_matrix_assemble(A);
```

#### 5.8.3 Associating Arrays

To associate the arrays in the BSC format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_bsc(LIS\_INT bnr, LIS\_INT bnc, LIS\_INT bnnz, LIS\_INT bptr[], LIS\_INT bindex[], LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_bsc(LIS\_INTEGER bnr, LIS\_INTEGER bnc, LIS\_INTEGER bnnz, LIS\_INTEGER bptr(), LIS\_INTEGER bindex(), LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

## 5.9 Variable Block Row (VBR)

The VBR format is the generalized version of the BSR format. The division points of the rows and columns are given by the arrays row and col. The VBR format stores the nonzero blocks (the blocks in which at least one nonzero element exists) in a format similar to that of CSR. Assume that nr and nc are the numbers of row and column divisions, respectively, and that bnnz denotes the number of nonzero blocks of A, and nnz denotes the total number of elements of the nonzero blocks. The VBR format uses six arrays, bptr, bindex, row, col, ptr, and value, to store data.

- row is an integer array of length nr + 1, which stores the starting row number of the block rows.
- col is an integer array of length nc + 1, which stores the starting column number of the block columns.
- bindex is an integer array of length *bnnz*, which stores the block column numbers of the nonzero blocks.
- bptr is an integer array of length nr + 1, which stores the starting points of the block rows in the array bindex.
- $\bullet$  value is a double precision array of length nnz, which stores the values of the elements of the nonzero blocks.
- ptr is an integer array of length bnnz + 1, which stores the starting points of the nonzero blocks in the array value.

## 5.9.1 Creating Matrices (for Serial and Multithreaded Environments)

The diagram on the right in Figure 20 shows how matrix A in Figure 20 is stored in the VBR format. A program to create the matrix in the VBR format is as follows:



Figure 20: Data structure of VBR format (for serial and multithreaded environments).

```
- For serial and multithreaded environments -
 1: LIS_INT n,nnz,nr,nc,bnnz;
2: LIS_INT *row,*col,*ptr,*bptr,*bindex;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
 5: n = 4; nnz = 11; bnnz = 6; nr = 3; nc = 3;
 6: bptr = (LIS_INT *)malloc( (nr+1)*sizeof(LIS_INT) );
           = (LIS_INT *)malloc( (nr+1)*sizeof(LIS_INT) );
8: col
           = (LIS_INT *)malloc( (nc+1)*sizeof(LIS_INT) );
           = (LIS_INT *)malloc( (bnnz+1)*sizeof(LIS_INT) );
9: ptr
10: bindex = (LIS_INT *)malloc( bnnz*sizeof(LIS_INT) );
11: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
12: lis_matrix_create(0,&A);
13: lis_matrix_set_size(A,0,n);
15: bptr[0] = 0; bptr[1] = 1; bptr[2] = 3; bptr[3] = 6;
16: row[0] = 0; row[1] = 1; row[2] = 3; row[3] = 4;
17: col[0] = 0; col[1] = 1; col[2] = 3; col[3] = 4;
18: bindex[0] = 0; bindex[1] = 0; bindex[2] = 1; bindex[3] = 0;
19: bindex[4] = 1; bindex[5] = 2;
20: ptr[0]
              = 0; ptr[1]
                               = 1; ptr[2]
                                               = 3; ptr[3]
                                                                   7;
                               = 10; ptr[6]
                                                = 11;
21: ptr[4]
              = 8; ptr[5]
22: value[0] = 11; value[1] = 21; value[2] = 0; value[3]
23: value[4] = 32; value[5] = 0; value[6] = 33; value[7]
24: value[8] = 0; value[9] = 43; value[10] = 44;
26: lis_matrix_set_vbr(nnz,nr,nc,bnnz,row,col,ptr,bptr,bindex,value,A);
27: lis_matrix_assemble(A);
```

## 5.9.2 Creating Matrices (for Multiprocessing Environment)

Figure 21 shows how matrix A in Figure 20 is stored in the VBR format on two processing elements. A program to create the matrix in the VBR format on two processing elements is as follows:



Figure 21: Data structure of VBR format (for multiprocessing environment).

```
- For multiprocessing environment
 1: LIS_INT n,nnz,nr,nc,bnnz,my_rank;
 2: LIS_INT *row,*col,*ptr,*bptr,*bindex;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
 6: if( my_rank==0 ) {n = 2; nnz = 7; bnnz = 3; nr = 2; nc = 3;}
                     {n = 2; nnz = 4; bnnz = 3; nr = 1; nc = 3;}
7: else
           = (LIS_INT *)malloc( (nr+1)*sizeof(LIS_INT) );
8: bptr
          = (LIS_INT *)malloc( (nr+1)*sizeof(LIS_INT) );
9: row
          = (LIS_INT *)malloc( (nc+1)*sizeof(LIS_INT) );
10: col
          = (LIS_INT *)malloc( (bnnz+1)*sizeof(LIS_INT) );
12: bindex = (LIS_INT *)malloc( bnnz*sizeof(LIS_INT) );
13: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
14: lis_matrix_create(MPI_COMM_WORLD,&A);
15: lis_matrix_set_size(A,n,0);
16: if( my_rank==0 ) {
        bptr[0] = 0; bptr[1] = 1; bptr[2] = 3;
17:
        row[0] = 0; row[1] = 1; row[2] = 3;
18:
        col[0] = 0; col[1] = 1; col[2] = 3; col[3] = 4;
19:
        bindex[0] = 0; bindex[1] = 0; bindex[2] = 1;
20:
                 = 0; ptr[1]
                               = 1; ptr[2]
                                                 = 3; ptr[3]
21:
        value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;
22:
23:
        value[4] = 32; value[5] = 0; value[6] = 33;}
24: else {
        bptr[0] = 0; bptr[1] = 3;
25:
        row[0] = 3; row[1] = 4;
26:
27:
        col[0] = 0; col[1] = 1; col[2] = 3; col[3] = 4;
28:
        bindex[0] = 0; bindex[1] = 1; bindex[2] = 2;
29:
        ptr[0]
                 = 0; ptr[1]
                                 = 1; ptr[2]
                                                 = 3; ptr[3]
        value[0] = 41; value[1] = 0; value[2] = 43; value[3] = 44;}
31: lis_matrix_set_vbr(nnz,nr,nc,bnnz,row,col,ptr,bptr,bindex,value,A);
32: lis_matrix_assemble(A);
```

## 5.9.3 Associating Arrays

To associate the arrays in the VBR format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_vbr(LIS\_INT nnz, LIS\_INT nr, LIS\_INT nc, LIS\_INT bnnz, LIS\_INT row[], LIS\_INT col[], LIS\_INT ptr[], LIS\_INT bptr[], LIS\_INT bindex[], LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_vbr(LIS\_INTEGER nnz, LIS\_INTEGER nr, LIS\_INTEGER nc, LIS\_INTEGER bnnz, LIS\_INTEGER row(), LIS\_INTEGER col(), LIS\_INTEGER ptr(), LIS\_INTEGER bptr(), LIS\_INTEGER bindex(), LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

# 5.10 Coordinate (COO)

The COO format uses three arrays row, col and value to store data.

- value is a double precision array of length nnz, which stores the values of the nonzero elements.
- row is an integer array of length nnz, which stores the row numbers of the nonzero elements.
- col is an integer array of length nnz, which stores the column numbers of the nonzero elements.

## 5.10.1 Creating Matrices (for Serial and Multithreaded Environments)

The diagram on the right in Figure 22 shows how matrix A in Figure 22 is stored in the COO format. A program to create the matrix in the COO format is as follows:

Figure 22: Data structure of COO format (for serial and multithreaded environments).

```
    For serial and multithreaded environments -

 1: LIS_INT n,nnz;
 2: LIS_INT *row,*col;
 3: LIS_SCALAR *value;
 4: LIS_MATRIX A;
5: n = 4; nnz = 8;
 6: row = (LIS_INT *)malloc( nnz*sizeof(LIS_INT) );
         = (LIS_INT *)malloc( nnz*sizeof(LIS_INT) );
8: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
9: lis_matrix_create(0,&A);
10: lis_matrix_set_size(A,0,n);
11:
12: row[0] = 0; row[1] = 1; row[2] = 3; row[3] = 1;
13: row[4] = 2; row[5] = 2; row[6] = 3; row[7] = 3;
14: col[0] = 0; col[1] = 0; col[2] = 0; col[3] = 1;
15: col[4] = 1; col[5] = 2; col[6] = 2; col[7] = 3;
16: value[0] = 11; value[1] = 21; value[2] = 41; value[3] = 22;
17: value[4] = 32; value[5] = 33; value[6] = 43; value[7] = 44;
19: lis_matrix_set_coo(nnz,row,col,value,A);
20: lis_matrix_assemble(A);
```

## 5.10.2 Creating Matrices (for Multiprocessing Environment)

Figure 23 shows how matrix A in Figure 22 is stored in the COO format on two processing elements. A program to create the matrix in the COO format on two processing elements is as follows:

0	1	1	3	2	2	3	3	A.row
0	0	1	0	1	2	2	3	A.col
11	21	22	41	32	33	43	44	A.value
PE0			PE	Ξ1				

Figure 23: Data structure of COO format (for multiprocessing environment).

```
- For multiprocessing environment -
 1: LIS_INT n,nnz,my_rank;
2: LIS_INT *row,*col;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
6: if( my_rank==0 ) {n = 2; nnz = 3;}
                     {n = 2; nnz = 5;}
7: else
         = (LIS_INT *)malloc( nnz*sizeof(LIS_INT) );
8: row
9: col = (LIS_INT *)malloc( nnz*sizeof(LIS_INT) );
10: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
11: lis_matrix_create(MPI_COMM_WORLD,&A);
12: lis_matrix_set_size(A,n,0);
13: if( my_rank==0 ) {
14:
        row[0] = 0; row[1] = 1; row[2] = 1;
15:
        col[0] = 0; col[1] = 0; col[2] = 1;
        value[0] = 11; value[1] = 21; value[2] = 22;}
16:
17: else {
18:
        row[0] = 3; row[1] = 2; row[2] = 2; row[3] = 3; row[4] = 3;
19:
        col[0] = 0; col[1] = 1; col[2] = 2; col[3] = 2; col[4] = 3;
        value[0] = 41; value[1] = 32; value[2] = 33; value[3] = 43; value[4] = 44;}
21: lis_matrix_set_coo(nnz,row,col,value,A);
22: lis_matrix_assemble(A);
```

## 5.10.3 Associating Arrays

To associate the arrays in the COO format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_coo(LIS\_INT nnz, LIS\_INT row[], LIS\_INT col[], LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_coo(LIS\_INTEGER nnz, LIS\_INTEGER row(), LIS\_INTEGER col(), LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

# 5.11 Dense (DNS)

The DNS format uses one array value to store data.

• value is a double precision array of length  $n \times n$ , which stores the values of the elements with priority given to the columns.

## 5.11.1 Creating Matrices (for Serial and Multithreaded Environments)

The right diagram in Figure 24 shows how matrix A in Figure 24 is stored in the DNS format. A program to create the matrix in the DNS format is as follows:

Figure 24: Data structure of DNS format (for serial and multithreaded environments).

```
To serial and multithreaded environments

1: LIS_INT n;

2: LIS_SCALAR *value;

3: LIS_MATRIX A;

4: n = 4;

5: value = (LIS_SCALAR *)malloc( n*n*sizeof(LIS_SCALAR) );

6: lis_matrix_create(0,&A);

7: lis_matrix_set_size(A,0,n);

8:

9: value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 41;

10: value[4] = 0; value[5] = 22; value[6] = 32; value[7] = 0;

11: value[8] = 0; value[9] = 0; value[10]= 33; value[11]= 43;

12: value[12]= 0; value[13]= 0; value[14]= 0; value[15]= 44;

13:

14: lis_matrix_set_dns(value,A);

15: lis_matrix_assemble(A);
```

## 5.11.2 Creating Matrices (for Multiprocessing Environment)

Figure 25 shows how matrix A in Figure 24 is stored in the DNS format on two processing elements. A program to create the matrix in the DNS format on two processing elements is as follows:



Figure 25: Data structure of DNS format (for multiprocessing environment).

```
- For multiprocessing environment -
 1: LIS_INT n,my_rank;
 2: LIS_SCALAR *value;
3: LIS_MATRIX A;
4: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
5: if( my_n = 0 ) n = 2;
                     {n = 2;}
6: else
7: value = (LIS_SCALAR *)malloc( n*n*sizeof(LIS_SCALAR) );
8: lis_matrix_create(MPI_COMM_WORLD,&A);
9: lis_matrix_set_size(A,n,0);
10: if( my_rank==0 ) {
11:
        value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;
        value[4] = 0; value[5] = 0; value[6] = 0; value[7] = 0;}
12:
13: else {
        value[0] = 0; value[1] = 41; value[2] = 32; value[3] = 0;
14:
        value[4] = 33; value[5] = 43; value[6] = 0; value[7] = 44;}
15:
16: lis_matrix_set_dns(value,A);
17: lis_matrix_assemble(A);
```

# 5.11.3 Associating Arrays

To associate the arrays in the DNS format with matrix A, the following functions are used:

- C LIS\_INT lis\_matrix\_set\_dns(LIS\_SCALAR value[], LIS\_MATRIX A)
- Fortran subroutine lis\_matrix\_set\_dns(LIS\_SCALAR value(), LIS\_MATRIX A, LIS\_INTEGER ierr)

# 6 Functions

This section describes the functions which can be employed by the user. The statuses of the solvers are defined as follows:

LIS\_SUCCESS(0) Normal termination

LIS\_ILL\_OPTION(1) Illegal option

LIS\_BREAKDOWN(2) Breakdown (division by zero)

LIS\_OUT\_OF\_MEMORY(3) Out of working memory

LIS\_MAXITER(4) Maximum number of iterations

LIS\_NOT\_IMPLEMENTED(5) Not implemented

LIS\_ERR\_FILE\_IO(6) File I/O error

# 6.1 Operating Vector Elements

Assume that the size of vector v is  $global\_n$  and that the size of the partial vectors stored on nprocs processing elements is  $local\_n$ .  $global\_n$  and  $local\_n$  are called the global size and the local size, respectively.

## 6.1.1 lis\_vector\_create

```
C LIS_INT lis_vector_create(LIS_Comm comm, LIS_VECTOR *v)
Fortran subroutine lis_vector_create(LIS_Comm comm, LIS_VECTOR v, LIS_INTEGER ierr)
```

## Description

Create vector v.

#### Input

comm The MPI communicator

## Output

v The vector

ierr The return code

#### Note

For the serial and multithreaded environments, the value of comm is ignored.

## 6.1.2 lis\_vector\_destroy

```
C LIS_INT lis_vector_destroy(LIS_VECTOR v)
Fortran subroutine lis_vector_destroy(LIS_VECTOR v, LIS_INTEGER ierr)
```

## Description

Destroy vector v.

## Input

v The vector to be destroyed

## Output

## 6.1.3 lis\_vector\_duplicate

```
C LIS_INT lis_vector_duplicate(void *vin, LIS_VECTOR *vout)
Fortran subroutine lis_vector_duplicate(LIS_VECTOR vin, LIS_VECTOR vout,
LIS_INTEGER ierr)
```

## Description

Create vector  $v_{out}$ , which has the same information as  $v_{in}$ .

## Input

vin The source vector or matrix

#### Output

vout The destination vector

ierr The return code

#### Note

The function lis\_vector\_duplicate does not copy the values, but allocates only the memory. To copy the values as well, the function lis\_vector\_copy must be called after this function.

### 6.1.4 lis\_vector\_set\_size

### Description

Assign the size of vector v.

### Input

v The vector

local\_n The size of the partial vector

global\_n The size of the global vector

Output

ierr The return code

#### Note

Either  $local_n$  or  $global_n$  must be provided.

For the serial and multithreaded environments,  $local_n$  is equal to  $global_n$ . Therefore, both  $lis_vector_set_size(v,n,0)$  and  $lis_vector_set_size(v,0,n)$  create a vector of size n.

For the multiprocessing environment,  $lis_vector_set_size(v,n,0)$  creates a partial vector of size n on each processing element. On the other hand,  $lis_vector_set_size(v,0,n)$  creates a partial vector of size  $m_p$  on processing element p. The values of  $m_p$  are determined by the library.

## 6.1.5 lis\_vector\_get\_size

## Description

Get the size of vector v.

#### Input

v The vector

#### Output

local\_n The size of the partial vector global\_n The size of the global vector

ierr The return code

## Note

For the serial and multithreaded environments, local\_n is equal to global\_n.

# 6.1.6 lis\_vector\_get\_range

```
C LIS_INT lis_vector_get_range(LIS_VECTOR v, LIS_INT *is, LIS_INT *ie)
Fortran subroutine lis_vector_get_range(LIS_VECTOR v, LIS_INTEGER is,
LIS_INTEGER ie, LIS_INTEGER ierr)
```

#### Description

Get the location of the partial vector v in the global vector.

#### Input

v The partial vector

#### Output

is The location where the partial vector v starts in the global vector ie The location where the partial vector v ends in the global vector

ierr The return code

#### Note

For the serial and multithreaded environments, a vector of size n results in is = 0 and ie = n in the C version, and is = 1 and ie = n + 1 in the Fortran version.

#### 6.1.7 lis\_vector\_set\_value

```
C LIS_INT lis_vector_set_value(LIS_INT flag, LIS_INT i, LIS_SCALAR value, LIS_VECTOR v)

Fortran subroutine lis_vector_set_value(LIS_INTEGER flag, LIS_INTEGER i, LIS_SCALAR value, LIS_VECTOR v, LIS_INTEGER ierr)
```

## Description

Assign the scalar value to the i-th row of vector v.

### Input

 $\mathtt{LIS\_INS\_VALUE} \ : \ v[i] = value$ 

 $\texttt{LIS\_ADD\_VALUE} : v[i] = v[i] + value$ 

i The location where the value is assigned

value The scalar value to be assigned

v The vector

#### Output

The vector with the scalar value assigned to the i-th row

ierr The return code

#### Note

For the multiprocessing environment, the i-th row of the global vector must be specified instead of the i-th row of the partial vector.

## 6.1.8 lis\_vector\_get\_value

## Description

Get the scalar value of the i-th row of vector v.

### Input

i The location where the value is assigned

v The source vector

## Output

value The value of the *i*-th row

ierr The return code

### Note

For the multiprocessing environment, the i-th row of the global vector must be specified.

## 6.1.9 lis\_vector\_set\_values

## Description

Assign scalar value[i] to the index[i]-th row of vector v, where i = 0, 1, ..., count - 1.

## Input

 $\texttt{flag} \qquad \qquad \texttt{LIS\_INS\_VALUE} \, : \, v[index[i]] = value[i]$ 

 $\texttt{LIS\_ADD\_VALUE} \ : \ v[index[i]] = v[index[i]] + value[i]$ 

The number of elements in the array that stores the scalar values

to be assigned

index The array that stores the location where the scalar values are as-

signed

value The array that stores the scalar values to be assigned

v The vector

Output

v The vector with scalar value[i] assigned to the index[i]-th row

ierr The return code

#### Note

For the multiprocessing environment, the index[i]-th row of the global vector must be specified instead of the index[i]-th row of the partial vector.

## 6.1.10 lis\_vector\_get\_values

```
C LIS_INT lis_vector_get_values(LIS_VECTOR v, LIS_INT start, LIS_INT count, LIS_SCALAR value[])
Fortran subroutine lis_vector_get_values(LIS_VECTOR v, LIS_INTEGER start, LIS_INTEGER count, LIS_SCALAR value(), LIS_INTEGER ierr)
```

#### Description

Get scalar value[i] of the start + i-th row of vector v, where i = 0, 1, ..., count - 1.

### Input

start The starting location

count The number of values to get

v The source vector

## Output

value The array to store the scalar values

ierr The return code

#### Note

For the multiprocessing environment, the start + i-th row of the global vector must be specified.

#### 6.1.11 lis\_vector\_scatter

#### Description

Assign scalar value[i] to the *i*-th row of vector v, where  $i = 0, 1, ..., global_n - 1$ .

## Input

value The array that stores the scalar values to be assigned

# Output

v The vector

ierr The return code

#### Note

## 6.1.12 lis\_vector\_gather

## Description

Get scalar value[i] of the *i*-th row of vector v, where  $i = 0, 1, ..., global_n - 1$ .

## Input

v The source vector

Output

value The array that stores the scalar values

ierr The return code

Note

## 6.1.13 lis\_vector\_is\_null

C LIS\_INT lis\_vector\_is\_null(LIS\_VECTOR v)
Fortran subroutine lis\_vector\_is\_null(LIS\_VECTOR v,LIS\_INTEGER ierr)

## Description

Determine if vector v is available.

## Input

v The vector

Output

ierr The return code

LIS\_TRUE Available
LIS\_FALSE Not available

# 6.2 Operating Matrix Elements

Assume that the size of matrix A is  $global\_n \times global\_n$  and that the size of each partial matrix stored on nprocs processing elements is  $local\_n \times global\_n$ . Here,  $global\_n$  and  $local\_n$  are called the number of rows of the global matrix and the number of rows of the partial matrix, respectively.

#### 6.2.1 lis\_matrix\_create

C LIS\_INT lis\_matrix\_create(LIS\_Comm comm, LIS\_MATRIX \*A)
Fortran subroutine lis\_matrix\_create(LIS\_Comm comm, LIS\_MATRIX A, LIS\_INTEGER ierr)

## Description

Create matrix A.

#### Input

comm The MPI communicator

## Output

A The matrix

ierr The return code

#### Note

For the serial and multithreaded environments, the value of comm is ignored.

#### 6.2.2 lis\_matrix\_destroy

C LIS\_INT lis\_matrix\_destroy(LIS\_MATRIX A)
Fortran subroutine lis\_matrix\_destroy(LIS\_MATRIX A, LIS\_INTEGER ierr)

## Description

Destroy matrix A.

## Input

A The matrix to be destroyed

## Output

ierr The return code

#### Note

The function  $lis_{matrix\_destroy}$  frees the memory for the set of arrays associated with matrix A.

## 6.2.3 lis\_matrix\_duplicate

## Description

Create matrix  $A_{out}$  which has the same information as  $A_{in}$ .

## Input

Ain The source matrix

Output

Aout The destination matrix

ierr The return code

#### Note

The function <code>lis\_matrix\_duplicate</code> does not copy the values of the elements of the matrix, but allocates only the memory. To copy the values of the elements as well, the function <code>lis\_matrix\_copy</code> must be called after this function.

#### 6.2.4 lis\_matrix\_malloc

## Description

Allocate memory for matrix A.

# Input

A The matrix

nnz\_row The average number of nonzero elements in each row

nnz The array of numbers of nonzero elements in each row

Output

ierr The return code

### Note

Either nnz\_row or nnz must be provided.

This function allocates memory for the function lis\_matrix\_set\_value.

#### 6.2.5 lis\_matrix\_set\_value

```
C LIS_INT lis_matrix_set_value(LIS_INT flag, LIS_INT i, LIS_INT j,
LIS_SCALAR value, LIS_MATRIX A)

Fortran subroutine lis_matrix_set_value(LIS_INTEGER flag, LIS_INTEGER i,
LIS_INTEGER j, LIS_SCALAR value, LIS_MATRIX A, LIS_INTEGER ierr)
```

#### Description

Assign the scalar value to the (i, j)-th element of matrix A.

## Input

flag	$\mathtt{LIS\_INS\_VALUE}  :  A[i,j] = value$
	$\mathtt{LIS\_ADD\_VALUE}  :  A[i,j] = A[i,j] + value$
i	The row number of the matrix
j	The column number of the matrix
value	The value to be assigned
A	The matrix

### Output

A The matrix

ierr The return code

#### Note

For the multiprocessing environment, the i-th row and the j-th column of the global matrix must be specified.

The function lis\_matrix\_set\_value stores the assigned value in a temporary internal format. Therefore, after lis\_matrix\_set\_value is called, the function lis\_matrix\_assemble must be called.

For large matrices, the introduction of the function <code>lis\_matrix\_set\_type</code> should be considered. See <code>lis-(\$VERSION)/test/test2.c</code> and <code>lis-(\$VERSION)/test/test2f.F90</code> for details.

#### 6.2.6 lis\_matrix\_assemble

```
C LIS_INT lis_matrix_assemble(LIS_MATRIX A)
Fortran subroutine lis_matrix_assemble(LIS_MATRIX A, LIS_INTEGER ierr)
```

## Description

Assemble matrix A into the specified storage format.

# Input

A The matrix

## Output

A The matrix assembled into the specified storage format

#### 6.2.7 lis\_matrix\_set\_size

```
C LIS_INT lis_matrix_set_size(LIS_MATRIX A, LIS_INT local_n,
LIS_INT global_n)

Fortran subroutine lis_matrix_set_size(LIS_MATRIX A, LIS_INTEGER local_n,
LIS_INTEGER global_n, LIS_INTEGER ierr)
```

#### Description

Assign the size of matrix A.

### Input

A The matrix

local\_n The number of rows of the partial matrix global\_n The number of rows of the global matrix

Output

ierr The return code

#### Note

Either  $local_n$  or  $global_n$  must be provided.

For the serial and multithreaded environments,  $local_n$  is equal to  $global_n$ . Therefore, both  $lis_matrix_set_size(A,n,0)$  and  $lis_matrix_set_size(A,0,n)$  create a matrix of size  $n \times n$ .

For the multiprocessing environment,  $lis_matrix_set_size(A,n,0)$  creates a partial matrix of size  $n \times N$  on each processing element, where N is the total sum of n. On the other hand,  $lis_matrix_set_size(A,0,n)$  creates a partial matrix of size  $m_p \times n$  on processing element p. The

lis\_matrix\_set\_size(A,0,n) creates a partial matrix of size  $m_p \times n$  on processing element p. T values of  $m_p$  are determined by the library.

## 6.2.8 lis\_matrix\_get\_size

```
C LIS_INT lis_matrix_get_size(LIS_MATRIX A, LIS_INT *local_n,
LIS_INT *global_n)
Fortran subroutine lis_matrix_get_size(LIS_MATRIX A, LIS_INTEGER local_n,
LIS_INTEGER global_n, LIS_INTEGER ierr)
```

#### Description

Get the size of matrix A.

#### Input

A The matrix

# Output

local\_n The number of rows of the partial matrix
global\_n The number of rows of the global matrix

ierr The return code

#### Note

For the serial and multithreaded environments, *local\_n* is equal to *global\_n*.

## 6.2.9 lis\_matrix\_get\_range

```
C LIS_INT lis_matrix_get_range(LIS_MATRIX A, LIS_INT *is, LIS_INT *ie)
Fortran subroutine lis_matrix_get_range(LIS_MATRIX A, LIS_INTEGER is,
LIS_INTEGER ie, LIS_INTEGER ierr)
```

#### Description

Get the location of partial matrix A in the global matrix.

## Input

A The partial matrix

## Output

is The location where partial matrix A starts in the global matrix

ie The location where partial matrix A ends in the global matrix

ierr The return code

#### Note

For the serial and multithreaded environments, a matrix of  $n \times n$  results in is = 0 and ie = n in the C version, and is = 1 and ie = n + 1 in the Fortran version.

## 6.2.10 lis\_matrix\_get\_nnz

## Description

Get the number of nonzero elements of matrix A.

## Input

A The matrix

## Output

nnz The number of nonzero elements

ierr The return code

### Note

For the multiprocessing environment, this function gets the number of nonzero elements of partial matrix A.

## 6.2.11 lis\_matrix\_set\_type

## Description

Assign the storage format.

## Input

A The matrix

matrix\_type The storage format

Output

ierr The return code

#### Note

 $\mathtt{matrix\_type}$  of A is  $\mathtt{LIS\_MATRIX\_CSR}$  when the matrix is created. The table below shows the available storage formats for  $\mathtt{matrix\_type}$ .

Storage format	matrix_type		
Compressed Sparse Row	(CSR)	{LIS_MATRIX_CSR 1}	
Compressed Sparse Column	(CSC)	{LIS_MATRIX_CSC 2}	
Modified Compressed Sparse Row	(MSR)	{LIS_MATRIX_MSR 3}	
Diagonal	(DIA)	{LIS_MATRIX_DIA 4}	
Ellpack-Itpack Generalized Diagonal	(ELL)	{LIS_MATRIX_ELL 5}	
Jagged Diagonal	(JAD)	{LIS_MATRIX_JAD 6}	
Block Sparse Row	(BSR)	{LIS_MATRIX_BSR 7}	
Block Sparse Column	(BSC)	{LIS_MATRIX_BSC 8}	
Variable Block Row	(VBR)	{LIS_MATRIX_VBR 9}	
Coordinate	(COO)	{LIS_MATRIX_COO 10}	
Dense	(DNS)	{LIS_MATRIX_DNS 11}	

## 6.2.12 lis\_matrix\_get\_type

## Description

Get the storage format.

## Input

A The matrix

Output

matrix\_type The storage format

#### 6.2.13 lis\_matrix\_set\_csr

## Description

Associate the arrays in the CSR format with matrix A.

#### Input

nnz The number of nonzero elements

ptr, index, value The arrays in the CSR format

A The matrix

#### Output

A The matrix associated with the arrays

#### Note

After lis\_matrix\_set\_csr is called, the function lis\_matrix\_assemble must be called. Array indexing must be zero-origin in the Fortran version.

## 6.2.14 lis\_matrix\_set\_csc

#### Description

Associate the arrays in the CSC format with matrix A.

## Input

nnz The number of nonzero elements

ptr, index, value The arrays in the CSC format

A The matrix

#### Output

A The matrix associated with the arrays

#### Note

After lis\_matrix\_set\_csc is called, the function lis\_matrix\_assemble must be called. Array indexing must be zero-origin in the Fortran version.

#### 6.2.15 lis\_matrix\_set\_msr

## Description

Associate the arrays in the MSR format with matrix A.

#### Input

nnz The number of nonzero elements

ndz The number of nonzero elements in the diagonal

index, value The arrays in the MSR format

A The matrix

#### Output

A The matrix associated with the arrays

#### Note

After lis\_matrix\_set\_msr is called, the function lis\_matrix\_assemble must be called. Array indexing must be zero-origin in the Fortran version.

#### 6.2.16 lis\_matrix\_set\_dia

#### Description

Associate the arrays in the DIA format with matrix A.

#### Input

nnd The number of nonzero diagonal elements

index, value The arrays in the DIA format

A The matrix

#### Output

A The matrix associated with the arrays

#### Note

After lis\_matrix\_set\_dia is called, the function lis\_matrix\_assemble must be called. Array indexing must be zero-origin in the Fortran version.

#### 6.2.17 lis\_matrix\_set\_ell

### Description

Associate the arrays in the ELL format with matrix A.

## Input

maxnzr The maximum number of nonzero elements in each row

index, value The arrays in the ELL format

A The matrix

## Output

A The matrix associated with the arrays

#### Note

After lis\_matrix\_set\_ell is called, the function lis\_matrix\_assemble must be called. Array indexing must be zero-origin in the Fortran version.

## 6.2.18 lis\_matrix\_set\_jad

### Description

Associate the arrays in the JAD format with matrix A.

## Input

nnz The number of nonzero elements

maxnzr The maximum number of nonzero elements in each row

A The matrix

### Output

A The matrix associated with the arrays

### Note

After lis\_matrix\_set\_jad is called, the function lis\_matrix\_assemble must be called. Array indexing must be zero-origin in the Fortran version.

#### 6.2.19 lis\_matrix\_set\_bsr

### Description

Associate the arrays in the BSR format with matrix A.

#### Input

bnr The row block size
bnc The column block size

bnnz The number of nonzero blocks
bptr, bindex, value The arrays in the BSR format

A The matrix

### Output

A The matrix associated with the arrays

#### Note

After lis\_matrix\_set\_bsr is called, the function lis\_matrix\_assemble must be called. Array indexing must be zero-origin in the Fortran version.

#### 6.2.20 lis\_matrix\_set\_bsc

```
C LIS_INT lis_matrix_set_bsc(LIS_INT bnr, LIS_INT bnc, LIS_INT bnnz, LIS_INT bptr[], LIS_INT bindex[], LIS_SCALAR value[], LIS_MATRIX A)

Fortran subroutine lis_matrix_set_bsc(LIS_INTEGER bnr, LIS_INTEGER bnc, LIS_INTEGER bnnz, LIS_INTEGER bptr(), LIS_INTEGER bindex(), LIS_SCALAR value(), LIS_MATRIX A, LIS_INTEGER ierr)
```

## Description

Associate the arrays in the BSC format with matrix A.

#### Input

bnr The row block size
bnc The column block size

bnnz The number of nonzero blocks
bptr, bindex, value The arrays in the BSC format

A The matrix

## Output

A The matrix associated with the arrays

### Note

After lis\_matrix\_set\_bsc is called, the function lis\_matrix\_assemble must be called. Array indexing must be zero-origin in the Fortran version.

#### 6.2.21 lis\_matrix\_set\_vbr

```
C LIS_INT lis_matrix_set_vbr(LIS_INT nnz, LIS_INT nr, LIS_INT nc,
    LIS_INT bnnz, LIS_INT row[], LIS_INT col[], LIS_INT ptr[],
    LIS_INT bptr[], LIS_INT bindex[], LIS_SCALAR value[],
    LIS_MATRIX A)

Fortran subroutine lis_matrix_set_vbr(LIS_INTEGER nnz, LIS_INTEGER nr,
    LIS_INTEGER nc, LIS_INTEGER bnnz, LIS_INTEGER row(),
    LIS_INTEGER col(), LIS_INTEGER ptr(), LIS_INTEGER bptr(),
    LIS_INTEGER bindex(), LIS_SCALAR value(), LIS_MATRIX A,
    LIS_INTEGER ierr)
```

### Description

Associate the arrays in the VBR format with matrix A.

## Input

nnz
The number of nonzero elements

The number of row blocks

The number of column blocks

The number of nonzero blocks

Tow, col, ptr, bptr, bindex, value The arrays in the VBR format

The matrix

## Output

A The matrix associated with the arrays

#### Note

After lis\_matrix\_set\_vbr is called, the function lis\_matrix\_assemble must be called. Array indexing must be zero-origin in the Fortran version.

## 6.2.22 lis\_matrix\_set\_coo

## Description

Associate the arrays in the COO format with matrix A.

## Input

nnz The number of nonzero elements

row, col, value The arrays in the COO format

A The matrix

## Output

A The matrix associated with the arrays

#### Note

After lis\_matrix\_set\_coo is called, the function lis\_matrix\_assemble must be called. Array indexing must be zero-origin in the Fortran version.

#### 6.2.23 lis\_matrix\_set\_dns

C LIS\_INT lis\_matrix\_set\_dns(LIS\_SCALAR value[], LIS\_MATRIX A)
Fortran subroutine lis\_matrix\_set\_dns(LIS\_SCALAR value(), LIS\_MATRIX A,
LIS\_INTEGER ierr)

#### Description

Associate the array in the DNS format with matrix A.

#### Input

value The array in the DNS format

A The matrix

#### Output

A The matrix associated with the array

#### Note

After lis\_matrix\_set\_dns is called, the function lis\_matrix\_assemble must be called. Array indexing must be zero-origin in the Fortran version.

#### 6.2.24 lis\_matrix\_unset

```
C LIS_INT lis_matrix_unset(LIS_MATRIX A)
Fortran subroutine lis_matrix_unset(LIS_MATRIX A, LIS_INTEGER ierr)
```

#### Description

Unassociate the arrays from matrix A without deallocating memory.

## Input

A The matrix associated with the arrays

#### Output

A The unassociated matrix

#### Note

After lis\_matrix\_unset is called, the function lis\_matrix\_destroy must be called.

# 6.3 Computing with Vectors and Matrices

## 6.3.1 lis\_vector\_swap

```
C LIS_INT lis_vector_swap(LIS_VECTOR x, LIS_VECTOR y)
Fortran subroutine lis_vector_swap(LIS_VECTOR x, LIS_VECTOR y, LIS_INTEGER ierr)
```

## Description

Swap the values of the vector elements.

## Input

x, y The source vectors

Output

x, y

The destination vectors

ierr The return code

# 6.3.2 lis\_vector\_copy

```
C LIS_INT lis_vector_copy(LIS_VECTOR x, LIS_VECTOR y)
Fortran subroutine lis_vector_copy(LIS_VECTOR x, LIS_VECTOR y, LIS_INTEGER ierr)
```

## Description

Copy the values of the vector elements.

## Input

x The source vector

Output

y The destination vector

## 6.3.3 lis\_vector\_axpy

C LIS\_INT lis\_vector\_axpy(LIS\_SCALAR alpha, LIS\_VECTOR x, LIS\_VECTOR y)
Fortran subroutine lis\_vector\_axpy(LIS\_SCALAR alpha, LIS\_VECTOR x, LIS\_VECTOR y,
LIS\_INTEGER ierr)

## Description

Calculate the sum of the vectors  $y = \alpha x + y$ .

## Input

alpha The scalar value

x, y The vectors

## Output

y  $\alpha x + y$  (vector y is overwritten)

ierr The return code

## 6.3.4 lis\_vector\_xpay

C LIS\_INT lis\_vector\_xpay(LIS\_VECTOR x, LIS\_SCALAR alpha, LIS\_VECTOR y)
Fortran subroutine lis\_vector\_xpay(LIS\_VECTOR x, LIS\_SCALAR alpha, LIS\_VECTOR y,
LIS\_INTEGER ierr)

## Description

Calculate the sum of the vectors  $y = x + \alpha y$ .

## Input

alpha The scalar value

x, y The vectors

# Output

y  $x + \alpha y$  (vector y is overwritten)

## 6.3.5 lis\_vector\_axpyz

C LIS\_INT lis\_vector\_axpyz(LIS\_SCALAR alpha, LIS\_VECTOR x, LIS\_VECTOR y, LIS\_VECTOR z)

Fortran subroutine lis\_vector\_axpyz(LIS\_SCALAR alpha, LIS\_VECTOR x, LIS\_VECTOR y, LIS\_VECTOR z, LIS\_INTEGER ierr)

## Description

Calculate the sum of the vectors  $z = \alpha x + y$ .

## Input

alpha The scalar value

x, y The vectors

## Output

 $\mathbf{z}$   $\alpha x + y$ 

ierr The return code

## 6.3.6 lis\_vector\_scale

## Description

Multiply vector x by scalar  $\alpha$ .

# ${\bf Input}$

alpha The scalar value

x The vector

## Output

 $\alpha x$  (vector x is overwritten)

## 6.3.7 lis\_vector\_pmul

C LIS\_INT lis\_vector\_pmul(LIS\_VECTOR x, LIS\_VECTOR y, LIS\_VECTOR z)
Fortran subroutine lis\_vector\_pmul(LIS\_VECTOR x, LIS\_VECTOR y, LIS\_VECTOR z,
LIS\_INTEGER ierr)

## Description

Multiply each element of vector x by the corresponding element of y.

## Input

x, y The vectors

## Output

 ${f z}$  The vector that stores the multiplied elements of x

ierr The return code

## 6.3.8 lis\_vector\_pdiv

C LIS\_INT lis\_vector\_pdiv(LIS\_VECTOR x, LIS\_VECTOR y, LIS\_VECTOR z)
Fortran subroutine lis\_vector\_pdiv(LIS\_VECTOR x, LIS\_VECTOR y, LIS\_VECTOR z,
LIS\_INTEGER ierr)

## Description

Divide each element of vector x by the corresponding element of y.

## Input

x, y The vectors

## Output

z The vector that stores the divided elements of x

## 6.3.9 lis\_vector\_set\_all

#### Description

Assign the scalar value to the elements of vector x.

## Input

value The scalar value to be assigned

x The vector

Output

x The vector with the value assigned to the elements

ierr The return code

## 6.3.10 lis\_vector\_abs

```
C LIS_INT lis_vector_abs(LIS_VECTOR x)
Fortran subroutine lis_vector_abs(LIS_VECTOR x, LIS_INTEGER ierr)
```

# Description

Get the absolute values of the elements of vector x.

## Input

x The vector

Output

x The vector that stores the absolute values

## 6.3.11 lis\_vector\_reciprocal

```
C LIS_INT lis_vector_reciprocal(LIS_VECTOR x)
Fortran subroutine lis_vector_reciprocal(LIS_VECTOR x, LIS_INTEGER ierr)
```

### Description

Get the reciprocal values of the elements of vector x.

## Input

x The vector

Output

x The vector that stores the reciprocal values

ierr The return code

## 6.3.12 lis\_vector\_conjugate

```
C LIS_INT lis_vector_conjugate(LIS_VECTOR x)
Fortran subroutine lis_vector_conjugate(LIS_VECTOR x, LIS_INTEGER ierr)
```

## Description

Get the conjugate complex values of the elements of vector x.

## Input

x The vector

Output

x The vector that stores the conjugate complex values

## 6.3.13 lis\_vector\_shift

## Description

Get the shifted values of the elements of vector x.

## Input

alpha The amount of the shift

x The vector

Output

x The vector that stores the shifted values

## 6.3.14 lis\_vector\_dot

### Description

Calculate the Hermitian inner product  $y^H x$ .

## Input

x, y The vectors

Output

value The inner product

ierr The return code

## $6.3.15 \quad lis\_vector\_nhdot$

## Description

Calculate the non-Hermitian inner product  $y^Tx$ .

## Input

x, y The vectors

Output

value The inner product

## 6.3.16 lis\_vector\_nrm1

C LIS\_INT lis\_vector\_nrm1(LIS\_VECTOR x, LIS\_SCALAR \*value)
Fortran subroutine lis\_vector\_nrm1(LIS\_VECTOR x, LIS\_SCALAR value, LIS\_INTEGER ierr)

## Description

Calculate the 1-norm of vector x.

## Input

x The vector

Output

value The 1-norm of the vector

ierr The return code

#### 6.3.17 lis\_vector\_nrm2

C LIS\_INT lis\_vector\_nrm2(LIS\_VECTOR x, LIS\_REAL \*value)
Fortran subroutine lis\_vector\_nrm2(LIS\_VECTOR x, LIS\_REAL value, LIS\_INTEGER ierr)

#### Description

Calculate the 2-norm of vector x.

#### Input

x The vector

Output

value The 2-norm of the vector

## 6.3.18 lis\_vector\_nrmi

C LIS\_INT lis\_vector\_nrmi(LIS\_VECTOR x, LIS\_SCALAR \*value)
Fortran subroutine lis\_vector\_nrmi(LIS\_VECTOR x, LIS\_SCALAR value, LIS\_INTEGER ierr)

## Description

Calculate the infinity norm of vector x.

## Input

x The vector

Output

value The infinity norm of the vector

ierr The return code

#### 6.3.19 lis\_vector\_sum

C LIS\_INT lis\_vector\_sum(LIS\_VECTOR x, LIS\_SCALAR \*value)
Fortran subroutine lis\_vector\_sum(LIS\_VECTOR x, LIS\_SCALAR value, LIS\_INTEGER ierr)

#### Description

Calculate the sum of the elements of vector x.

#### Input

x The vector

Output

value The sum of the vector elements

### 6.3.20 lis\_matrix\_set\_blocksize

C LIS\_INT lis\_matrix\_set\_blocksize(LIS\_MATRIX A, LIS\_INT bnr, LIS\_INT bnc, LIS\_INT row[], LIS\_INT col[])
Fortran subroutine lis\_matrix\_set\_blocksize(LIS\_MATRIX A, LIS\_INTEGER bnr, LIS\_INTEGER bnc, LIS\_INTEGER row[], LIS\_INTEGER col[], LIS\_INTEGER ierr)

# Description

Assign the block size of the BSR, BSC, and VBR formats.

# Input

The row block size of the BSR (BSC) format or the number of row blocks of the VBR format  The olumn block size of the BSR (BSC) format or the number of column blocks of the VBR format  The array of the row division information about the VBR format  The array of the column division information about the VBR format	A	The matrix
column blocks of the VBR format  row The array of the row division information about the VBR format  col The array of the column division information about the VBR for-	bnr	
The array of the column division information about the VBR for-	bnc	,
·	row	The array of the row division information about the VBR format
	col	·

# Output

### 6.3.21 lis\_matrix\_convert

# Description

Convert matrix  $A_{in}$  into  $A_{out}$  of the format specified by lis\_matrix\_set\_type.

Input

Ain The source matrix

Output

Aout The destination matrix

ierr The return code

#### Note

The storage format of  $A_{out}$  is set by lis\_matrix\_set\_type. The block size of the BSR, BSC, and VBR formats is set by lis\_matrix\_set\_blocksize. See lis-(\$VERSION)/test/test2.c and lis-(\$VERSION)/test/test2f.F90.

The conversions indicated by 1 in the table below are performed directly, and the others are performed via the indicated formats. The conversions with no indication are performed via the CSR format.

Src \Dst	CSR	CSC	MSR	DIA	ELL	JAD	BSR	BSC	VBR	COO	DNS
CSR		1	1	1	1	1	1	CSC	1	1	1
COO	1	1	1	CSR	CSR	CSR	CSR	CSC	CSR		CSR

# 6.3.22 lis\_matrix\_copy

# Description

Copy the values of the matrix elements.

# Input

Ain The source matrix

Output

Aout The destination matrix

ierr The return code

### 6.3.23 lis\_matrix\_axpy

C LIS\_INT lis\_matrix\_axpy(LIS\_SCALAR alpha, LIS\_MATRIX A, LIS\_MATRIX B)
Fortran subroutine lis\_matrix\_axpy(LIS\_SCALAR alpha, LIS\_MATRIX A, LIS\_MATRIX B,
LIS\_INTEGER ierr)

### Description

Calculate the sum of the matrices  $B = \alpha A + B$ .

### Input

alpha The scalar value

A, B The matrices

Output

B  $\alpha A + B$  (matrix B is overwritten)

ierr The return code

Matrices  $A,\,B$  must be in the DNS format.

# 6.3.24 lis\_matrix\_xpay

C LIS\_INT lis\_matrix\_xpay(LIS\_SCALAR alpha, LIS\_MATRIX A, LIS\_MATRIX B)
Fortran subroutine lis\_matrix\_xpay(LIS\_SCALAR alpha, LIS\_MATRIX A, LIS\_MATRIX B,
LIS\_INTEGER ierr)

### Description

Calculate the sum of the matrices  $B = A + \alpha B$ .

### Input

alpha The scalar value

A, B The matrices

Output

B  $A + \alpha B$  (matrix B is overwritten)

ierr The return code

#### Note

Matrices A, B must be in the DNS format.

# $6.3.25 \quad lis\_matrix\_axpyz$

C LIS\_INT lis\_matrix\_axpyz(LIS\_SCALAR alpha, LIS\_MATRIX A, LIS\_MATRIX B, LIS\_MATRIX C)

Fortran subroutine lis\_matrix\_axpyz(LIS\_SCALAR alpha, LIS\_MATRIX A, LIS\_MATRIX B, LIS\_MATRIX C, LIS\_INTEGER ierr)

# Description

Calculate the sum of the matrices  $C = \alpha A + B$ .

# Input

alpha The scalar value

A, B The matrices

Output

 $\mathbf{C}$   $\alpha A + B$ 

ierr The return code

#### Note

Matrices A, B, and C must be in the DNS format.

### 6.3.26 lis\_matrix\_scale

C LIS\_INT lis\_matrix\_scale(LIS\_MATRIX A, LIS\_VECTOR b, LIS\_VECTOR d, LIS\_INT action)

Fortran subroutine lis\_matrix\_scale(LIS\_MATRIX A, LIS\_VECTOR b, LIS\_VECTOR d, LIS\_INTEGER action, LIS\_INTEGER ierr)

### Description

Scale matrix A and vector b.

### Input

A The matrix
b The vector

action LIS\_SCALE\_JACOBI : Jacobi scaling  $D^{-1}Ax = D^{-1}b$ , where D rep-

resents the diagonal of  $A = (a_{ij})$ 

LIS\_SCALE\_SYMM\_DIAG : Diagonal scaling  $D^{-1/2}AD^{-1/2}x=D^{-1/2}b$ , where  $D^{-1/2}$  represents a diagonal matrix with  $1/\sqrt{a_{ii}}$  as the

diagona

Output

A The scaled matrix

b The scaled vector

d The vector that stores the diagonal elements of  $D^{-1}$  or  $D^{-1/2}$ 

# 6.3.27 lis\_matrix\_get\_diagonal

C LIS\_INT lis\_matrix\_get\_diagonal(LIS\_MATRIX A, LIS\_VECTOR d)
Fortran subroutine lis\_matrix\_get\_diagonal(LIS\_MATRIX A, LIS\_VECTOR d,
LIS\_INTEGER ierr)

# Description

Store the diagonal elements of matrix A to vector d.

# Input

A The matrix

# Output

d The vector that stores the diagonal elements of the matrix

ierr The return code

### 6.3.28 lis\_matrix\_shift\_diagonal

### Description

Shift the diagonal of matrix A.

### Input

alpha The amount of the shift

A The matrix

### Output

A The shifted matrix

### 6.3.29 lis\_matvec

C LIS\_INT lis\_matvec(LIS\_MATRIX A, LIS\_VECTOR x, LIS\_VECTOR y)
Fortran subroutine lis\_matvec(LIS\_MATRIX A, LIS\_VECTOR x, LIS\_VECTOR y,
LIS\_INTEGER ierr)

### Description

Calculate the matrix-vector product y = Ax.

# Input

A The matrix

x The vector

### Output

 $\mathbf{y}$  Ax

ierr The return code

# 6.3.30 lis\_matvect

C LIS\_INT lis\_matvect(LIS\_MATRIX A, LIS\_VECTOR x, LIS\_VECTOR y)
Fortran subroutine lis\_matvect(LIS\_MATRIX A, LIS\_VECTOR x, LIS\_VECTOR y,
LIS\_INTEGER ierr)

# Description

Calculate the matrix-vector product  $y = A^T x$ .

### Input

A The matrix

x The vector

# Output

 $\mathbf{y}$   $A^T x$ 

# 6.4 Solving Linear Equations

### 6.4.1 lis\_solver\_create

C LIS\_INT lis\_solver\_create(LIS\_SOLVER \*solver)
Fortran subroutine lis\_solver\_create(LIS\_SOLVER solver, LIS\_INTEGER ierr)

### Description

Create the solver.

### Input

None

# Output

solver The solver

ierr The return code

### Note

solver has the information on the solver, the preconditioner, etc.

### 6.4.2 lis\_solver\_destroy

C LIS\_INT lis\_solver\_destroy(LIS\_SOLVER solver)
Fortran subroutine lis\_solver\_destroy(LIS\_SOLVER solver, LIS\_INTEGER ierr)

### Description

Destroy the solver.

### Input

solver The solver to be destroyed

# Output

# 6.4.3 lis\_precon\_create

C LIS\_INT lis\_precon\_create(LIS\_SOLVER solver, LIS\_PRECON \*precon)
Fortran subroutine lis\_precon\_create(LIS\_SOLVER solver, LIS\_PRECON precon,
LIS\_INTEGER ierr)

# Description

Create the preconditioner.

# Input

None

# Output

solver The solver

precon The preconditioner

ierr The return code

# ${\bf 6.4.4 \quad lis\_precon\_destroy}$

C LIS\_INT lis\_precon\_destroy(LIS\_PRECON precon)
Fortran subroutine lis\_precon\_destroy(LIS\_PRECON precon, LIS\_INTEGER ierr)

### Description

Destroy the preconditioner.

# Input

precon The preconditioner to be destroyed

# Output

# 6.4.5 lis\_solver\_set\_option

# Description

Set the options for the solver.

# Input

text The command line options

# Output

solver The solver

ierr The return code

#### Note

The table below shows the available command line options, where  $-i \{cg|1\}$  means -i cg or -i 1 and -maxiter [1000] indicates that -maxiter defaults to 1,000.

Options for Linear Solvers (Default: -i bicg)

Solver	Option	Auxiliary Options	<u> </u>
CG	-i {cg 1}	J 21	
$\operatorname{BiCG}$	-i {bicg 2}		
CGS	-i {cgs 3}		
BiCGSTAB	-i {bicgstab 4}		
BiCGSTAB(l)	-i {bicgstabl 5}	-ell [2]	The degree $l$
GPBiCG	-i {gpbicg 6}		
TFQMR	-i {tfqmr 7}		
Orthomin(m)	-i {orthomin 8}	-restart [40]	The restart value $m$
GMRES(m)	-i {gmres 9}	-restart [40]	The restart value $m$
Jacobi	-i {jacobi 10}		
Gauss-Seidel	-i {gs 11}		
SOR	-i {sor 12}	-omega [1.9]	The relaxation coefficient
			$\omega \ (0 < \omega < 2)$
BiCGSafe	-i {bicgsafe 13}		
$\operatorname{CR}$	-i {cr 14}		
$\operatorname{BiCR}$	-i {bicr 15}		
CRS	-i {crs 16}		
BiCRSTAB	-i {bicrstab 17}		
GPBiCR	-i {gpbicr 18}		
BiCRSafe	-i {bicrsafe 19}		
FGMRES(m)	-i {fgmres 20}	-restart [40]	The restart value $m$
IDR(s)	-i {idrs 21}	-irestart [2]	The restart value $s$
IDR(1)	-i {idr1 22}		
MINRES	-i {minres 23}		
COCG	-i {cocg 24}		
COCR	-i {cocr 25}		

Options for Preconditioners (Default: -p none)

Preconditioner	Option	Auxiliary Options	
None	-p {none 0}		
Jacobi	-p {jacobi 1}		
ILU(k)	-p {ilu 2}	-ilu_fill [0]	The fill level $k$
SSOR	-p {ssor 3}	-ssor_omega [1.0]	The relaxation coefficient
			$\omega \ (0 < \omega < 2)$
Hybrid	-p {hybrid 4}	-hybrid_i [sor]	The linear solver
		-hybrid_maxiter [25]	The maximum number of iterations
		-hybrid_tol [1.0e-3]	The convergence tolerance
		-hybrid_omega [1.5]	The relaxation coefficient $\omega$
			of the SOR $(0 < \omega < 2)$
		-hybrid_ell [2]	The degree $l$ of the BiCGSTAB(l)
		-hybrid_restart [40]	The restart values
			of the GMRES and Orthomin
I+S	-p {is 5}	-is_alpha [1.0]	The parameter $\alpha$ of $I + \alpha S^{(m)}$
		-is_m [3]	The parameter $m$ of $I + \alpha S^{(m)}$
SAINV	-p {sainv 6}	-sainv_drop [0.05]	The drop criterion
SA-AMG	-p {saamg 7}	-saamg_unsym [false]	Select the unsymmetric version
			(The matrix structure must be
			symmetric)
		-saamg_theta [0.05 0.12]	The drop criterion $a_{ij}^2 \le \theta^2  a_{ii}   a_{jj} $
			(symmetric or unsymmetric)
Crout ILU	-p {iluc 8}	-iluc_drop [0.05]	The drop criterion
		-iluc_rate [5.0]	The ratio of the maximum fill-in
ILUT	-p {ilut 9}		
Additive	-adds true	-adds_iter [1]	The number of iterations
Schwarz			

# Other Options

Option				
-maxiter [1000]	The maximum number of iterations			
-tol [1.0e-12]	The convergence tolerance tol			
-tol_w [1.0]	The convergence tolerance $tol_w$			
-print [0]	The output of the residual history			
	-print {none 0}	None		
	-print {mem 1}	Save the residual history		
	-print {out 2}	Output it to the standard output		
	-print {all 3}	Save the residual history and output it		
		to the standard output		
-scale [0]	The scaling			
	(The result will overwi	rite the original matrix and vectors)		
	-scale {none 0}	No scaling		
	-scale {jacobi 1}			
		(D represents the diagonal of $A = (a_{ij})$ )		
	-scale {symm_diag 2	?} The diagonal scaling $D^{-1/2}AD^{-1/2}x = D^{-1/2}b$		
		$(D^{-1/2}$ represents the diagonal matrix		
		with $1/\sqrt{a_{ii}}$ as the diagonal)		
<pre>-initx_zeros [1]</pre>	The behavior of the in	· · · · · · · · · · · · · · · · · · ·		
	-initx_zeros {false			
		of the function lis_solve()		
	-initx_zeros {true	-		
-conv_cond [0]	The convergence condi			
	-conv_cond {nrm2_r			
		1} $  b - Ax  _2 \le tol *   b  _2$		
	-conv_cond {nrm1_b 2} $  b - Ax  _1 \le tol_w *   b  _1 + tol_w$			
-omp_num_threads [t]	The number of threads			
	(t represents the maximum number of threads)			
-storage [0]	The matrix storage format			
-storage_block [2]	The block size of the BSR and BSC formats			
-f [0] The precision of the linear solver				
	-f {double 0} Double precision  f {quad   1} Double double (quad qual quad qual quad qual quad qual quad quad qual quad quad quad quad quad quad quad quad			
	-f {quad 1}	Double-double (quadruple) precision		

# 6.4.6 lis\_solver\_set\_optionC

```
C LIS_INT lis_solver_set_optionC(LIS_SOLVER solver)
Fortran subroutine lis_solver_set_optionC(LIS_SOLVER solver, LIS_INTEGER ierr)
```

#### Description

Set the options for the solver on the command line.

#### Input

None

### Output

 ${\tt solver} \hspace{1cm} {\tt The \ solver}$ 

ierr The return code

#### 6.4.7 lis\_solve

```
C LIS_INT lis_solve(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x,
LIS_SOLVER solver)

Fortran subroutine lis_solve(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x,
LIS_SOLVER solver, LIS_INTEGER ierr)
```

# Description

Solve the linear equation Ax = b with the specified solver.

#### Input

A The coefficient matrix

b The right-hand side vector

x The initial vector

solver The solver

#### Output

x The solution

The number of iterations, the execution time, etc.

ierr The return code

#### Note

If the option  $-initx\_zeros$  {false|0} is specified, the initial vector is given by the argument x. Otherwise, all the components of the initial vector are set to 0.

This function returns 0 if the status of the solver (solver->retcode) is LIS\_BREAKDOWN or LIS\_MAXITER. See also the function lis\_solver\_get\_status().

#### 6.4.8 lis\_solve\_kernel

```
C LIS_INT lis_solve_kernel(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x,
LIS_SOLVER solver, LIS_PRECON, precon)

Fortran subroutine lis_solve_kernel(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x,
LIS_SOLVER solver, LIS_PRECON precon, LIS_INTEGER ierr)
```

#### Description

Solve the linear equation Ax = b with the specified solver and the predefined preconditioner.

### Input

A The coefficient matrix

b The right-hand side vector

x The initial vector

solver The solver

precon The preconditioner

Output

x The solution

The number of iterations, the execution time, etc.

ierr The return code

#### Note

See lis-(\$VERSION)/src/esolver/lis\_esolver\_ii.c, which computes the smallest eigenvalue by calling lis\_solve\_kernel multiple times, for example.

This function returns 0 if the status of the solver (solver->retcode) is LIS\_BREAKDOWN or LIS\_MAXITER. See also the function lis\_solver\_get\_status().

# 6.4.9 lis\_solver\_get\_status

C LIS\_INT lis\_solver\_get\_status(LIS\_SOLVER solver, LIS\_INT \*status)
Fortran subroutine lis\_solver\_get\_status(LIS\_SOLVER solver, LIS\_INTEGER status,
LIS\_INTEGER ierr)

# Description

Get the status from the solver.

# Input

solver The solver

Output

status The status

ierr The return code

#### Note

This function returns the status of the solver (solver->retcode).

# 6.4.10 lis\_solver\_get\_iter

### Description

Get the number of iterations from the solver.

#### Input

solver The solver

Output

iter The number of iterations

# 6.4.11 lis\_solver\_get\_iterex

### Description

Get the detailed information on the number of iterations from the solver.

#### Input

solver The solver

### Output

iter The number of iterations

iter\_double The number of double precision iterations

iter\_quad The number of double-double (quadruple) precision iterations

ierr The return code

### 6.4.12 lis\_solver\_get\_time

#### Description

Get the execution time from the solver.

# Input

solver The solver

### Output

time The time in seconds of the execution

### 6.4.13 lis\_solver\_get\_timeex

```
C LIS_INT lis_solver_get_timeex(LIS_SOLVER solver, double *time, double *time, double *ptime, double *pc_time, double *p_i_time)

Fortran subroutine lis_solver_get_timeex(LIS_SOLVER solver, real*8 time, real*8 itime, real*8 ptime, real*8 p_c_time, real*8 p_i_time, LIS_INTEGER ierr)
```

#### Description

Get the detailed information on the execution time from the solver.

#### Input

solver The solver

Output

time The total time in seconds

itime The time in seconds of the iterations

ptime The time in seconds of the preconditioning

p\_c\_time The time in seconds of the creation of the preconditioner

p\_i\_time The time in seconds of the iterations in the preconditioner

ierr The return code

#### 6.4.14 lis\_solver\_get\_residualnorm

#### Description

Get the relative residual norm  $||b - Ax||_2/||b||_2$  from the solver.

#### Input

solver The solver

Output

residual The relative residual norm  $||b - Ax||_2/||b||_2$ 

# 6.4.15 lis\_solver\_get\_rhistory

```
C LIS_INT lis_solver_get_rhistory(LIS_SOLVER solver, LIS_VECTOR v)
Fortran subroutine lis_solver_get_rhistory(LIS_SOLVER solver, LIS_VECTOR v,
LIS_INTEGER ierr)
```

# Description

Get the residual history from the solver.

# Input

solver The solver

Output

v The vector

ierr The return code

#### Note

Vector v must be created in advance with the function  $lis_vector_create$ . When vector v is shorter than the residual history, it stores the residual history in order to vector v.

# 6.4.16 lis\_solver\_get\_solver

C LIS\_INT lis\_solver\_get\_solver(LIS\_SOLVER solver, LIS\_INT \*nsol)
Fortran subroutine lis\_solver\_get\_solver(LIS\_SOLVER solver, LIS\_INTEGER nsol,
LIS\_INTEGER ierr)

# Description

Get the solver number from the solver.

# Input

solver The solver

Output

nsol The solver number ierr The return code

### 6.4.17 lis\_solver\_get\_precon

# Description

Get the preconditioner number from the solver.

### Input

solver The solver

Output

precon\_type The preconditioner number

# 6.4.18 lis\_solver\_get\_solvername

# Description

Get the solver name from the solver number.

# Input

nsol The solver number

# Output

 $\begin{array}{ccc} {\tt name} & & {\tt The \ solver \ name} \\ {\tt ierr} & & {\tt The \ return \ code} \end{array}$ 

### 6.4.19 lis\_solver\_get\_preconname

### Description

Get the preconditioner name from the preconditioner number.

### Input

precon\_type The preconditioner number

### Output

name The preconditioner name

# 6.5 Solving Eigenvalue Problems

# $\bf 6.5.1 \quad lis\_esolver\_create$

C LIS\_INT lis\_esolver\_create(LIS\_ESOLVER \*esolver)
Fortran subroutine lis\_esolver\_create(LIS\_ESOLVER esolver, LIS\_INTEGER ierr)

### Description

Create the eigensolver.

### Input

None

# Output

esolver The eigensolver ierr The return code

### Note

esolver has the information on the eigensolver, the preconditioner, etc.

### 6.5.2 lis\_esolver\_destroy

C LIS\_INT lis\_esolver\_destroy(LIS\_ESOLVER esolver)
Fortran subroutine lis\_esolver\_destroy(LIS\_ESOLVER esolver, LIS\_INTEGER ierr)

# Description

Destroy the eigensolver.

### Input

esolver The eigensolver to be destoyed

### Output

# 6.5.3 lis\_esolver\_set\_option

# Description

Set the options for the eigensolver.

# Input

text The command line options

# Output

esolver The eigensolver ierr The return code

#### Note

The table below shows the available command line options, where -e {pi|1} means -e pi or -e 1 and -emaxiter [1000] indicates that -emaxiter defaults to 1,000.

Options for Eigensolvers (Default: -e cr)

Eigensolver	Option	Auxiliary Options	,
Power	-e {pi 1}		
Inverse	-e {ii 2}	-i [bicg]	The linear solver
Rayleigh Quotient	-e {rqi 3}	-i [bicg]	The linear solver
$\overline{CG}$	-e {cg 4}	-i [cg]	The linear solver
CR	-e {cr 5}	-i [bicg]	The linear solver
Subspace	-e {si 6}	-ss [1]	The size of the subspace
Lanczos	-e {li 7}	-ss [1]	The size of the subspace
Arnoldi	-e {ai 8}	-ss [1]	The size of the subspace
Generalized Power	-e {gpi 9}	-i [bicg]	The linear solver
Generalized Inverse	-e {gii 10}	-i [bicg]	The linear solver
Generalized Rayleigh Quotient	-e {grqi 11}	-i [bicg]	The linear solver
Generalized CG	-e {gcg 12}	-i [cg]	The linear solver
Generalized CR	-e {gcr 13}	-i [bicg]	The linear solver
Generalized Subspace	-e {gsi 14}	-ss [1]	The size of the subspace
Generalized Lanczos	-e {gli 15}	-ss [1]	The size of the subspace
Generalized Arnoldi	-e {gai 16}	-ss [1]	The size of the subspace

Options for Preconditioners (Default: -p none)

Preconditioner	Option	Auxiliary Options	
None	-p {none 0}		
Jacobi	-p {jacobi 1}		
ILU(k)	-p {ilu 2}	-ilu_fill [0]	The fill level $k$
SSOR	-p {ssor 3}	-ssor_omega [1.0]	The relaxation coefficient
			$\omega \ (0 < \omega < 2)$
Hybrid	-p {hybrid 4}	-hybrid_i [sor]	The linear solver
		-hybrid_maxiter [25]	The maximum number of iterations
		-hybrid_tol [1.0e-3]	The convergence tolerance
		-hybrid_omega [1.5]	The relaxation coefficient $\omega$
			of the SOR $(0 < \omega < 2)$
		-hybrid_ell [2]	The degree $l$ of the BiCGSTAB(l)
		-hybrid_restart [40]	The restart values
			of the GMRES and Orthomin
I+S	-p {is 5}	-is_alpha [1.0]	The parameter $\alpha$ of $I + \alpha S^{(m)}$
		-is_m [3]	The parameter $m$ of $I + \alpha S^{(m)}$
SAINV	-p {sainv 6}	-sainv_drop [0.05]	The drop criterion
SA-AMG	-p {saamg 7}	-saamg_unsym [false]	Select the unsymmetric version
			(The matrix structure must be
			symmetric)
		-saamg_theta [0.05 0.12]	The drop criterion $a_{ij}^2 \le \theta^2  a_{ii}   a_{jj} $
			(symmetric or unsymmetric)
Crout ILU	-p {iluc 8}	-iluc_drop [0.05]	The drop criterion
		-iluc_rate [5.0]	The ratio of the maximum fill-in
ILUT	-p {ilut 9}		
Additive	-adds true	-adds_iter [1]	The number of iterations
Schwarz			

# Other Options

Option				
-emaxiter [1000]	The maximum number of iterations			
-etol [1.0e-12]	The convergence tolerance			
-eprint [0]	The output of the residual history			
	-eprint {none 0}	None		
	-eprint {mem 1}	Save the residual history		
	-eprint {out 2}	Output it to the standard output		
	-eprint {all 3}	Save the residual history and output it		
		to the standard output		
-ie [ii]	-ie [ii] The inner eigensolver used in Subspace, Lanczos, and Arnoldi			
-ige [gii]	The inner eigensolver used in Generalized Subspace, Generalized Lanczos,			
	and Generalized Arnoldi			
-shift [0.0]	The amount of the real part of the shift $\sigma$			
-shift_im [0.0]	The amount of the imag	ginary part of the shift $\sigma$		
-initx_ones [1]	The behavior of the init	ial vector $x_0$		
	-initx_ones {false 0	Components are given by the argument $x$		
		of the function lis_esolve()		
	-initx_ones {true 1}	All the components are set to 1		
-omp_num_threads [t]	The number of threads			
	(t represents the maximum number of threads)			
-estorage [0]	The matrix storage format			
-estorage_block [2]	The block size of the BSR and BSC formats			
-ef [0]	The precision of the eigensolver			
	-ef {double 0}	Double precision		
	-ef {quad 1}	Double-double (quadruple) precision		

### 6.5.4 lis\_esolver\_set\_optionC

```
C LIS_INT lis_esolver_set_optionC(LIS_ESOLVER esolver)
Fortran subroutine lis_esolver_set_optionC(LIS_ESOLVER esolver, LIS_INTEGER ierr)
```

#### Description

Set the options for the eigensolver on the command line.

#### Input

None

### Output

esolver The eigensolver ierr The return code

#### 6.5.5 lis\_esolve

# Description

Solve the standard eigenvalue problem  $Ax = \lambda x$  with the specified eigensolver.

#### Input

A The matrix

x The initial vector

esolver The eigensolver

### Output

evalue The eigenvalue of mode 0

x The associated eigenvector

esolver The number of iterations, the execution time, etc.

ierr The return code

#### Note

If the option  $-initx_ones$  {false|0} is specified, the initial vector is given by the argument x. Otherwise, all the components of the initial vector are set to 1.

This function returns 0 if the status of the eigensolver (esolver->retcode) is LIS\_MAXITER. See also the function lis\_esolver\_get\_status().

# 6.5.6 lis\_gesolve

```
C LIS_INT lis_gesolve(LIS_MATRIX A, LIS_MATRIX B,
LIS_VECTOR x, LIS_REAL evalue, LIS_ESOLVER esolver)

Fortran subroutine lis_gesolve(LIS_MATRIX A, LIS_MATRIX B,
LIS_VECTOR x, LIS_REAL evalue, LIS_ESOLVER esolver, LIS_INTEGER ierr)
```

#### Description

Solve the generalized eigenvalue problem  $Ax = \lambda Bx$  with the specified eigensolver.

The eigensolver

#### Input

A The matrix

B The matrix

The initial vector

### Output

esolver

evalue The eigenvalue of mode 0

x The associated eigenvector

esolver The number of iterations, the execution time, etc.

ierr The return code

#### Note

If the option  $-initx_ones$  {false|0} is specified, the initial vector is given by the argument x. Otherwise, all the components of the initial vector are set to 1.

This function returns 0 if the status of the eigensolver (esolver->retcode) is LIS\_MAXITER. See also the function lis\_esolver\_get\_status().

# 6.5.7 lis\_esolver\_get\_status

C LIS\_INT lis\_esolver\_get\_status(LIS\_ESOLVER esolver, LIS\_INT \*status)
Fortran subroutine lis\_esolver\_get\_status(LIS\_ESOLVER esolver, LIS\_INTEGER status,
LIS\_INTEGER ierr)

### Description

Get the status for the specified eigenpair from the eigensolver.

# Input

esolver The eigensolver

Output

status The status

ierr The return code

#### Note

This function returns the status of the eigensolver (esolver->retcode).

# ${\bf 6.5.8 \quad lis\_esolver\_get\_iter}$

#### Description

Get the number of iterations for the specified eigenpair from the eigensolver.

### Input

esolver The eigensolver

Output

iter The number of iterations

# 6.5.9 lis\_esolver\_get\_iterex

### Description

Get the detailed information on the number of iterations for the specified eigenpair from the eigensolver.

### Input

esolver The eigensolver

### Output

iter The number of iterations

iter\_double The number of double precision iterations

iter\_quad The number of double-double (quadruple) precision iterations

ierr The return code

# 6.5.10 lis\_esolver\_get\_time

### Description

Get the execution time for the specified eigenpair from the eigensolver.

#### Input

esolver The eigensolver

#### Output

time The time in seconds of the execution

### 6.5.11 lis\_esolver\_get\_timeex

```
C LIS_INT lis_esolver_get_timeex(LIS_ESOLVER esolver, double *time, double *time, double *ptime, double *ptime, double *ptime, double *ptime, double *ptime)

Fortran subroutine lis_esolver_get_timeex(LIS_ESOLVER esolver, real*8 time, real*8 itime, real*8 ptime, real*8 p_c_time, real*8 p_i_time, LIS_INTEGER ierr)
```

#### Description

Get the detailed information on the execution time for the specified eigenpair from the eigensolver.

### Input

esolver The eigensolver

Output

time The total time in seconds

itime The time in seconds of the iterations

ptime The time in seconds of the preconditioning

p\_c\_timeThe time in seconds of the creation of the preconditionerp\_i\_timeThe time in seconds of the iterations in the preconditioner

ierr The return code

#### 6.5.12 lis\_esolver\_get\_residualnorm

### Description

Get the relative residual norm  $||\lambda x - (B^{-1})Ax||_2/||\lambda x||_2$  for the specified eigenpair from the eigensolver.

### Input

esolver The eigensolver

Output

residual norm  $||\lambda x - Ax||_2/||\lambda x||_2$ 

# 6.5.13 lis\_esolver\_get\_rhistory

```
C LIS_INT lis_esolver_get_rhistory(LIS_ESOLVER esolver, LIS_VECTOR v)
Fortran subroutine lis_esolver_get_rhistory(LIS_ESOLVER esolver, LIS_VECTOR v,
LIS_INTEGER ierr)
```

### Description

Get the residual history for the specified eigenpair from the eigensolver.

### Input

esolver The eigensolver

Output

v The vector

ierr The return code

#### Note

Vector v must be created in advance with the function  $lis_vector_create$ . When vector v is shorter than the residual history, it stores the residual history in order to vector v.

### 6.5.14 lis\_esolver\_get\_evalues

# Description

Get all the eigenvalues from the eigensolver.

# Input

esolver The eigensolver

Output

v The vector which stores the eigenvalues

ierr The return code

### Note

Vector v must be created in advance with the function lis\_vector\_create.

### 6.5.15 lis\_esolver\_get\_evectors

#### Description

Get all the eigenvectors from the eigensolver.

### Input

esolver The eigensolver

Output

M The matrix in the COO format which stores the eigenvectors

ierr The return code

#### Note

Matrix M must be created in advance with the function  $lis_matrix_create$ .

# $\bf 6.5.16 \quad lis\_esolver\_get\_residual norms$

#### Description

Get the relative residual norms  $||\lambda x - (B^{-1})Ax||_2/||\lambda x||_2$  of all the eigenpairs from the eigensolver.

#### Input

esolver The eigensolver

Output

v The vector which stores the residual norms

ierr The return code

#### Note

Vector v must be created in advance with the function  $lis_vector_create$ .

### 6.5.17 lis\_esolver\_get\_iters

#### Description

Get the numbers of iterations of all the eigenpairs from the eigensolver.

#### Input

esolver The eigensolver

Output

v The vector which stores the numbers of iterations

ierr The return code

Note

Vector v must be created in advance with the function lis\_vector\_create.

### 6.5.18 lis\_esolver\_get\_esolver

### Description

Get the eigensolver number from the eigensolver.

#### Input

esolver The eigensolver

Output

nesol The eigensolver number

ierr The return code

#### 6.5.19 lis\_esolver\_get\_esolvername

### Description

Get the eigensolver name from the eigensolver number.

# Input

nesol The eigensolver number

Output

ename The eigensolver name
ierr The return code

# 6.6 Computing with Arrays

The following functions, which are not parallelized, are for local processing. Array data are stored in column-major order. Array indexing is zero-origin. See lis-(\$VERSION)/test/test6.c and lis-(\$VERSION)/test/test6f.F90.

### 6.6.1 lis\_array\_swap

#### Description

Swap the values of the vector elements.

### Input

n The size of the vectors

x, y The source arrays that store vectors x, y of size n

### Output

x, y The destination arrays

ierr The return code

# 6.6.2 lis\_array\_copy

#### Description

Copy the values of the vector elements.

#### Input

n The size of the vectors

 ${\tt x}$  The source array that stores vector x

#### Output

y The destination array

# 6.6.3 lis\_array\_axpy

C LIS\_INT lis\_array\_axpy(LIS\_INT n, LIS\_SCALAR alpha, LIS\_SCALAR x[], LIS\_SCALAR y[])

Fortran subroutine lis\_array\_axpy(LIS\_INTEGER n, LIS\_SCALAR alpha, LIS\_SCALAR x(), LIS\_SCALAR y(), LIS\_INTEGER ierr)

### Description

Calculate the sum of the vectors  $y = \alpha x + y$ .

#### Input

n The size of the vectors

alpha The scalar value

x, y The arrays that store vectors x, y

### Output

y  $\alpha x + y$  (vector y is overwritten)

ierr The return code

# 6.6.4 lis\_array\_xpay

C LIS\_INT lis\_array\_xpay(LIS\_INT n, LIS\_SCALAR x[], LIS\_SCALAR alpha, LIS\_SCALAR y[])

Fortran subroutine lis\_array\_xpay(LIS\_INTEGER n, LIS\_SCALAR x(), LIS\_SCALAR alpha, LIS\_SCALAR y(), LIS\_INTEGER ierr)

### Description

Calculate the sum of the vectors  $y = x + \alpha y$ .

#### Input

n The size of the vectors

alpha The scalar value

x, y The arrays that store vectors x, y

# Output

y  $x + \alpha y$  (vector y is overwritten)

# $6.6.5 \quad lis\_array\_axpyz$

### Description

Calculate the sum of the vectors  $z = \alpha x + y$ .

#### Input

n The size of the vectors

alpha The scalar value

x, y The arrays that store vectors x, y

### Output

z  $\alpha x + y$ 

ierr The return code

### 6.6.6 lis\_array\_scale

### Description

Multiply vector x by scalar  $\alpha$ .

# Input

n The size of the vector

alpha The scalar value

 $\mathbf{x}$  The array that stores vector x

### Output

 $\alpha x$  (vector x is overwritten)

# 6.6.7 lis\_array\_pmul

```
C LIS_INT lis_array_pmul(LIS_INT n, LIS_SCALAR x[], LIS_SCALAR y[],
LIS_SCALAR z[])

Fortran subroutine lis_array_pmul(LIS_INTEGER n, LIS_SCALAR x(), LIS_SCALAR y(),
LIS_SCALAR z(), LIS_INTEGER ierr)
```

#### Description

Multiply each element of vector x by the corresponding element of y.

#### Input

n The size of the vectors

x, y The arrays that store vectors x, y

# Output

z The array that stores the multiplied elements of x

ierr The return code

# 6.6.8 lis\_array\_pdiv

```
C LIS_INT lis_array_pdiv(LIS_INT n, LIS_SCALAR x[], LIS_SCALAR y[],
LIS_SCALAR z[])

Fortran subroutine lis_array_pdiv(LIS_INTEGER n, LIS_SCALAR x(), LIS_SCALAR y(),
LIS_SCALAR z(), LIS_INTEGER ierr)
```

# Description

Divide each element of vector x by the corresponding element of y.

### Input

n The size of the vectors

x, y The arrays that store vectors x, y

#### Output

z The array that stores the divided elements of x

## 6.6.9 lis\_array\_set\_all

#### Description

Assign the scalar value to the elements of vector x.

## Input

n The size of the vector

value The scalar value to be assigned

 $\mathbf{x}$  The array that stores vector  $\mathbf{x}$ 

#### Output

The array with the value assigned to the elements

ierr The return code

### 6.6.10 lis\_array\_abs

```
C LIS_INT lis_array_abs(LIS_INT n, LIS_SCALAR x[])
Fortran subroutine lis_array_abs(LIS_INTEGER n, LIS_SCALAR x(), LIS_INTEGER ierr)
```

#### Description

Get the absolute values of the elements of vector x.

### Input

n The size of the vector

 $\mathbf{x}$  The array that stores vector  $\mathbf{x}$ 

### Output

**x** The array that stores the absolute values

## 6.6.11 lis\_array\_reciprocal

```
C LIS_INT lis_array_reciprocal(LIS_INT n, LIS_SCALAR x[])
Fortran subroutine lis_array_reciprocal(LIS_INTEGER n, LIS_SCALAR x(),
LIS_INTEGER ierr)
```

## Description

Get the reciprocal values of the elements of vector x.

## Input

n The size of the vector

 $\mathbf{x}$  The array that stores vector  $\mathbf{x}$ 

#### Output

x The array that stores the reciprocal values

ierr The return code

## ${\bf 6.6.12}\quad {\bf lis\_array\_conjugate}$

### Description

Get the conjugate values of the elements of vector x.

## Input

n The size of the vector

 $\mathbf{x}$  The array that stores vector x

### Output

x The array that stores the conjugate values

## 6.6.13 lis\_array\_shift

### Description

Get the shifted values of the elements of vector x.

## Input

n The size of the vector

alpha The amount of the shift

 $\mathbf{x}$  The array that stores vector  $\mathbf{x}$ 

#### Output

x The array that stores the shifted values

ierr The return code

### 6.6.14 lis\_array\_dot

C LIS\_INT lis\_array\_dot(LIS\_INT n, LIS\_SCALAR x[], LIS\_SCALAR y[], LIS\_SCALAR \*value)

Fortran subroutine lis\_array\_dot(LIS\_INTEGER n, LIS\_SCALAR x(), LIS\_SCALAR y(), LIS\_SCALAR value, LIS\_INTEGER ierr)

#### Description

Calculate the Hermitian inner product  $y^H x$  of vectors x, y.

### Input

n The size of the vectors

 ${\tt x}$ ,  ${\tt y}$  The arrays that store vectors x,y

## Output

value The Hermitian inner product

## 6.6.15 lis\_array\_nhdot

C LIS\_INT lis\_array\_nhdot(LIS\_INT n, LIS\_SCALAR x[], LIS\_SCALAR y[], LIS\_SCALAR \*value)

Fortran subroutine lis\_array\_nhdot(LIS\_INTEGER n, LIS\_SCALAR x(), LIS\_SCALAR y(), LIS\_SCALAR value, LIS\_INTEGER ierr)

#### Description

Calculate the non-Hermitian inner product  $y^T x$  of vectors x, y.

#### Input

n The size of the vectors

x, y The arrays that store vectors x, y

Output

value The non-Hermitian inner product

ierr The return code

# 6.6.16 lis\_array\_nrm1

#### Description

Calculate the 1-norm of vector x.

### Input

n The size of the vector

 $\mathbf{x}$  The array that stores vector  $\mathbf{x}$ 

Output

value The 1-norm of the vector

## 6.6.17 lis\_array\_nrm2

## Description

Calculate the 2-norm of vector x.

## Input

n The size of the vector

 $\mathbf{x}$  The array that stores vector  $\mathbf{x}$ 

Output

value The 2-norm of the vector

ierr The return code

## 6.6.18 lis\_array\_nrmi

### Description

Calculate the infinity norm of vector x.

## Input

n The size of the vector

 $\mathbf{x}$  The array that stores vector x

Output

value The infinity norm of the vector

## 6.6.19 lis\_array\_sum

## Description

Calculate the sum of the elements of vector x.

# Input

n The size of the vector

 $\mathbf{x}$  The array that stores vector x

Output

value The sum of the vector elements

## 6.6.20 lis\_array\_matvec

#### Description

Calculate the matrix-vector product Ax.

#### Input

n The size of the matrix and vectors

The array that stores matrix A of size  $n \times n$ 

 $\mathbf{x}$  The array that stores vector x of size n

The array that stores vector y of size n

op LIS\_INS\_VALUE : y = Ax

 $\mathtt{LIS\_SUB\_VALUE} \, : \, y = y - Ax$ 

#### Output

У

ierr The return code

#### 6.6.21 lis\_array\_matvect

```
C LIS_INT lis_array_matvect(LIS_INT n, LIS_SCALAR a[], LIS_SCALAR x[], LIS_SCALAR y[], LIS_INT op)

Fortran subroutine lis_array_matvect(LIS_INTEGER n, LIS_SCALAR a(), LIS_SCALAR x(), LIS_SCALAR y(), LIS_INTEGER op, LIS_INTEGER ierr)
```

## Description

Calculate the matrix-vector product  $A^Tx$ .

## Input

n The size of the matrix and vectors

a The array that stores matrix A of size  $n \times n$ 

 $\mathbf{x}$  The array that stores vector x of size n

The array that stores vector y of size n

op LIS\_INS\_VALUE :  $y = A^T x$ 

 $\mathtt{LIS\_SUB\_VALUE} \, : \, y = y - A^T x$ 

## Output

y y

## 6.6.22 lis\_array\_matvec\_ns

```
C LIS_INTEGER lis_array_matvec_ns(LIS_INT m, LIS_INT n, LIS_SCALAR a[],
LIS_INT lda, LIS_SCALAR x[], LIS_SCALAR y[], LIS_INT op)

Fortran subroutine lis_array_matvec_ns(LIS_INTEGER m, LIS_INTEGER n, LIS_SCALAR a()
LIS_INTEGER lda, LIS_SCALAR x(), LIS_SCALAR y(), LIS_INTEGER op,
LIS_INTEGER ierr)
```

### Description

Calculate the matrix-vector product Ax, where matrix A is not square.

## Input

m, n	The sizes of the matrix and vectors
a	The array that stores matrix $A$ of size $m \times n$
lda	The size of the leading dimension of array ${\cal A}$
x	The array that stores vector $x$ of size $n$
У	The array that stores vector $y$ of size $m$
ор	${\tt LIS\_INS\_VALUE}:y=Ax$
	$\mathtt{LIS\_SUB\_VALUE}  :  y = y - Ax$

# Output

У	y

## 6.6.23 lis\_array\_matmat

```
C LIS_INT lis_array_matmat(LIS_INT n, LIS_SCALAR a[], LIS_SCALAR b[],
    LIS_SCALAR c[], LIS_INT op)

Fortran subroutine lis_array_matmat(LIS_INTEGER n, LIS_SCALAR a(), LIS_SCALAR b(),
    LIS_SCALAR c(), LIS_INTEGER op, LIS_INTEGER ierr)
```

# Description

Calculate the matrix-matrix product AB.

# Input

n	The size of the matrices
a	The array that stores matrix $A$ of size $n \times n$
b	The array that stores matrix $B$ of size $n \times n$
С	The array that stores matrix $C$ of size $n \times n$
ор	${\tt LIS\_INS\_VALUE}:C=AB$
	LIS_SUB_VALUE : $C = C - AB$

# Output

 $\mathsf{c}$ 

## 6.6.24 lis\_array\_matmat\_ns

```
C LIS_INT lis_array_matmat_ns(LIS_INT 1, LIS_INT m, LIS_INT n,
LIS_SCALAR a[], LIS_INT lda, LIS_SCALAR b[], LIS_INT ldb, LIS_SCALAR c[],
LIS_INT ldc, LIS_INT op)

Fortran subroutine lis_array_matmat_ns(LIS_INTEGER 1, LIS_INTEGER m, LIS_INTEGER n,
LIS_SCALAR a(), LIS_INTEGER lda, LIS_SCALAR b(), LIS_INTEGER ldb,
LIS_SCALAR c(), LIS_INTEGER ldc, LIS_INTEGER op, LIS_INTEGER ierr)
```

### Description

Calculate the matrix-matrix product AB, where matrices A,B are not square.

## Input

m, n	The sizes of the matrices
a	The array that stores matrix $A$ of size $l \times m$
lda	The size of the leading dimension of array ${\cal A}$
b	The array that stores matrix $B$ of size $m \times n$
ldb	The size of the leading dimension of array ${\cal B}$
С	The array that stores matrix $C$ of size $l \times n$
ldc	The size of the leading dimension of array ${\cal C}$
ор	${\tt LIS\_INS\_VALUE}  :  C = AB$
	${\tt LIS\_SUB\_VALUE}:C=C-AB$
<b>.</b>	

## Output

 $\mathsf{c}$ 

## 6.6.25 lis\_array\_ge

```
C LIS_INT lis_array_ge(LIS_INT n, LIS_SCALAR a[])
Fortran subroutine lis_solve(LIS_INTEGER n, LIS_SCALAR a(), LIS_INTEGER ierr)
```

### Description

Calculate the inverse of matrix A with the Gaussian elimination.

#### Input

n The size of the matrix

The array that stores matrix A of size  $n \times n$ 

## Output

a The inverse  $A^{-1}$  ierr The return code

#### 6.6.26 lis\_array\_solve

```
C LIS_INT lis_array_solve(LIS_INT n, LIS_SCALAR a[], LIS_SCALAR b[],
LIS_SCALAR x[], LIS_SCALAR w[])

Fortran subroutine lis_array_solve(LIS_INTEGER n, LIS_SCALAR a(), LIS_SCALAR b(),
LIS_SCALAR x(), LIS_SCALAR w(), LIS_INTEGER ierr)
```

#### Description

Solve the linear equation Ax = b with the direct method.

# Input

n The size of the matrix

The array that stores coefficient matrix A of size  $n \times n$ 

b The array that stores right-hand side vector b of size n

 $\mathbf{w}$  The work array of size  $n \times n$ 

## Output

 $\mathbf{x}$  The array that stores solution x

## 6.6.27 lis\_array\_cgs

```
C LIS_INT lis_array_cgs(LIS_INT n, LIS_SCALAR a[], LIS_SCALAR q[],
LIS_SCALAR r[])
Fortran subroutine lis_array_cgs(LIS_INTEGER n, LIS_SCALAR a(), LIS_SCALAR q(),
LIS_SCALAR r(), LIS_INTEGER ierr)
```

#### Description

Calculate the QR factorization QR = A with the classical Gram-Schmidt process.

#### Input

n The size of the matrices

a The array that stores matrix A of size  $n \times n$ 

## Output

**q** The array that stores orthogonal matrix Q of size  $n \times n$ 

The array that stores upper-triangular matrix R of size  $n \times n$ 

ierr The return code

### 6.6.28 lis\_array\_mgs

```
C LIS_INT lis_array_mgs(LIS_INT n, LIS_SCALAR a[], LIS_SCALAR q[],
LIS_SCALAR r[])

Fortran subroutine lis_array_mgs(LIS_INTEGER n, LIS_SCALAR a(), LIS_SCALAR q(),
LIS_SCALAR r(), LIS_INTEGER ierr)
```

#### Description

Calculate the QR factorization QR = A with the modified Gram-Schmidt process.

## Input

n The size of the matrices

a The array that stores matrix A of size  $n \times n$ 

#### Output

**q** The array that stores orthogonal matrix Q of size  $n \times n$ 

The array that stores upper-triangular matrix R of size  $n \times n$ 

## 6.6.29 lis\_array\_qr

```
С
       LIS_INT lis_array_qr(LIS_INT n, LIS_SCALAR a[], LIS_SCALAR q[],
         LIS_SCALAR r[], LIS_INT *qriter, LIS_REAL *qrerr)
Fortran subroutine lis_array_qr(LIS_INTEGER n, LIS_SCALAR a(), LIS_SCALAR q(),
         LIS_SCALAR r(), LIS_INTEGER qriter, LIS_REAL qrerr, LIS_INTEGER ierr)
```

# Description

Calculate the eigenvalues of matrix A with the QR algorithm.

# 1

ierr

Input	
n	The size of the matrices
a	The array that stores symmetric matrix $A$ of size $n \times n$
q	The work array of size $n \times n$
r	The work array of size $n \times n$
Output	
a	The array that stores the block upper-triangular matrix with eigenvalues in the block diagonal elements after similarity transformation
qriter	The number of iterations of the QR algorithm
qrerr	The 2-norm of the first subdiagonal element $A(2,1)$ after similarity transformation

The return code

# 6.7 Operating External Files

## 6.7.1 lis\_input

### Description

Read the matrix and vector data from the external file.

### Input

filename The source file

### Output

A The matrix in the specified storage format

b The right-hand side vector

x The solution

ierr The return code

#### Note

The following file formats are supported:

- $\bullet$  The extended Matrix Market format (extended to allow vector data)
- $\bullet\,$  The Harwell-Boeing format

## 6.7.2 lis\_input\_vector

### Description

Read the vector data from the external file.

## Input

filename The source file

### Output

v The vector

ierr The return code

#### Note

The following file formats are supported:

- $\bullet\,$  The PLAIN format
- The extended Matrix Market format (extended to allow vector data)

## 6.7.3 lis\_input\_matrix

### Description

Read the matrix data from the external file.

### Input

filename The source file

### Output

A The matrix in the specified storage format

x The solution

ierr The return code

#### Note

The following file formats are supported:

- The Matrix Market format
- The Harwell-Boeing format

### 6.7.4 lis\_output

```
C LIS_INT lis_output(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x,
LIS_INT format, char *filename)

Fortran subroutine lis_output(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x,
LIS_INTEGER format, character filename, LIS_INTEGER ierr)
```

## Description

Write the matrix and vector data into the external file.

## Input

A The matrix

b The right-hand side vector

x The solution

format The file format

LIS\_FMT\_MM The Matrix Market format

filename The destination file

Output

ierr The return code

## Note

In the C version, NULL can be input if the vector should not be written to the external file.

## 6.7.5 lis\_output\_vector

### Description

Write the vector data into the external file.

## Input

v The vector

format The file format

LIS\_FMT\_PLAIN The PLAIN format

LIS\_FMT\_MM The Matrix Market format

filename The destination file

Output

ierr The return code

## 6.7.6 lis\_output\_matrix

## Description

Write the matrix data into the external file.

### Input

A The matrix

format The file format

LIS\_FMT\_MM The Matrix Market format

filename The destination file

Output

# 6.8 Other Functions

## 6.8.1 lis\_initialize

```
C LIS_INT lis_initialize(LIS_INT* argc, char** argv[])
Fortran subroutine lis_initialize(LIS_INTEGER ierr)
```

## Description

Initialize the execution environment.

Input

argc The number of command line arguments

argv The command line argument

Output

ierr The return code

## 6.8.2 lis\_finalize

```
C LIS_INT lis_finalize()
Fortran subroutine lis_finalize(LIS_INTEGER ierr)
```

## Description

Finalize the execution environment.

### Input

None

## Output

### 6.8.3 lis\_wtime

```
C double lis_wtime()
Fortran function lis_wtime()
```

## Description

Measure the elapsed time.

## Input

None

### Output

The elapsed time in seconds from the given point is returned as the double precision number.

### Note

To measure the processing time, call <code>lis\_wtime</code> to get the starting time, call it again to get the ending time, and calculate the difference.

#### **6.8.4** CHKERR

```
C void CHKERR(LIS_INT ierr)
Fortran subroutine CHKERR(LIS_INTEGER ierr)
```

#### Description

Check the value of the return code.

### Input

ierr

The return code

### Output

None

#### Note

If the value of the return code is not 0, it calls lis\_finalize and terminates the program.

# $\bf 6.8.5 \quad lis\_printf$

C LIS\_INT lis\_printf(LIS\_Comm comm, const char \*mess, ...)

# Description

Print message on processing element 0.

Input

comm The MPI communicator

Output

mess The message

Note

The string '%D' is replaced with '%lld' if LIS\_INT is long long int, and is replaced with '%d' if it is int.

For the serial and multithreaded environments, the value of comm is ignored.

# References

- [1] A. Nishida. Experience in Developing an Open Source Scalable Software Infrastructure in Japan. Lecture Notes in Computer Science 6017, pp. 87-98, Springer, 2010.
- [2] M. R. Hestenes and E. Stiefel. Methods of Conjugate Gradients for Solving Linear Systems. Journal of Research of the National Bureau of Standards, Vol. 49, No. 6, pp. 409–436, 1952.
- [3] C. Lanczos. Solution of Linear Equations by Minimized Iterations. Journal of Research of the National Bureau of Standards, Vol. 49, No. 1, pp. 33–53, 1952.
- [4] R. Fletcher. Conjugate Gradient Methods for Indefinite Systems. Lecture Notes in Mathematics 506, pp. 73–89, Springer, 1976.
- [5] T. Sogabe, M. Sugihara, and S. Zhang. An Extension of the Conjugate Residual Method to Non-symmetric Linear Systems. Journal of Computational and Applied Mathematics, Vol. 226, No. 1, pp. 103–113, 2009.
- [6] P. Sonneveld. CGS, A Fast Lanczos-Type Solver for Nonsymmetric Linear Systems. SIAM Journal on Scientific and Statistical Computing, Vol. 10, No. 1, pp. 36–52, 1989.
- [7] K. Abe, T. Sogabe, S. Fujino, and S. Zhang. A Product-Type Krylov Subspace Method Based on Conjugate Residual Method for Nonsymmetric Coefficient Matrices (in Japanese). IPSJ Transactions on Advanced Computing Systems, Vol. 48, No. SIG8(ACS18), pp. 11–21, 2007.
- [8] H. van der Vorst. Bi-CGSTAB: A Fast and Smoothly Converging Variant of Bi-CG for the Solution of Nonsymmetric Linear Systems. SIAM Journal on Scientific and Statistical Computing, Vol. 13, No. 2, pp. 631–644, 1992.
- [9] S. Zhang. Generalized Product-Type Methods Preconditionings Based on Bi-CG for Solving Nonsymmetric Linear Systems. SIAM Journal on Scientific Computing, Vol. 18, No. 2, pp. 537–551, 1997.
- [10] S. Fujino, M. Fujiwara, and M. Yoshida. A Proposal of Preconditioned BiCGSafe Method with Safe Convergence. Proceedings of The 17th IMACS World Congress on Scientific Computation, Applied Mathematics and Simulation, CD-ROM, 2005.
- [11] S. Fujino and Y. Onoue. Estimation of BiCRSafe Method Based on Residual of BiCR Method (in Japanese). IPSJ SIG Technical Report, 2007-HPC-111, pp. 25–30, 2007.
- [12] G. L. G. Sleijpen, H. A. van der Vorst, and D. R. Fokkema. BiCGstab(l) and Other Hybrid Bi-CG Methods. Numerical Algorithms, Vol. 7, No. 1, pp. 75–109, 1994.
- [13] R. W. Freund. A Transpose-Free Quasi-Minimal Residual Algorithm for Non-Hermitian Linear Systems. SIAM Journal on Scientific Computing, Vol. 14, No. 2, pp. 470–482, 1993.
- [14] K. R. Biermann. Eine unveröffentlichte Jugendarbeit C. G. J. Jacobi über wiederholte Funktionen. Journal für die reine und angewandte Mathematik, Vol. 207, pp. 996-112, 1961.
- [15] S. C. Eisenstat, H. C. Elman, and M. H. Schultz. Variational Iterative Methods for Nonsymmetric Systems of Linear Equations. SIAM Journal on Numerical Analysis, Vol. 20, No. 2, pp. 345–357, 1983.
- [16] C. F. Gauss. Theoria Motus Corporum Coelestium in Sectionibus Conicis Solem. Perthes et Besser, 1809.
- [17] L. Seidel. Über ein Verfahren, die Gleichungen, auf welche die Methode der kleinsten Quadrate führt, sowie lineäre Gleichungen überhaupt, durch successive Annäherung aufzulösen. Abhandlungen der Bayerischen Akademie, Vol. 11, pp. 81–108, 1873.

- [18] Y. Saad and M. H. Schultz. GMRES: A Generalized Minimal Residual Algorithm for Solving Non-symmetric Linear Systems. SIAM Journal on Scientific and Statistical Computing, Vol. 7, No. 3, pp. 856–869, 1986.
- [19] D. M. Young. Iterative Methods for Solving Partial Difference Equations of Elliptic Type. Doctoral Thesis, Harvard University, 1950.
- [20] S. P. Frankel. Convergence Rates of Iterative Treatments of Partial Differential Equations. Mathematical Tables and Other Aids to Computation, Vol. 4, No. 30, pp. 65–75, 1950.
- [21] Y. Saad. A Flexible Inner-outer Preconditioned GMRES Algorithm. SIAM Journal on Scientific and Statistical Computing, Vol. 14, No. 2, pp. 461–469, 1993.
- [22] P. Sonnerveld and M. B. van Gijzen. IDR(s): a Family of Simple and Fast Algorithms for Solving Large Nonsymmetric Systems of Linear Equations. SIAM Journal on Scientific Computing, Vol. 31, No. 2, pp. 1035–1062, 2008.
- [23] C. C. Paige and M. A. Saunders. Solution of Sparse Indefinite Systems of Linear Equations. SIAM Journal on Numerical Analysis, Vol. 12, No. 4, pp. 617–629, 1975.
- [24] H. A. van der Vorst and J. B. M. Melissen. A Petrov-Galerkin Type Method for Solving Ax = b, where A is Symmetric Complex. IEEE Transactions on Magnetics, Vol. 26, No. 2, pp. 706–708, 1990.
- [25] T. Sogabe and S. Zhang. A COCR Method for Solving Complex Symmetric Linear Systems. Journal of Computational and Applied Mathematics, Vol. 199, No. 2, pp. 297–303, 2007.
- [26] R. von Mises and H. Pollaczek-Geiringer. Praktische Verfahren der Gleichungsauflösung. Zeitschrift für Angewandte Mathematik und Mechanik, Vol. 9, No. 2, pp. 152–164, 1929.
- [27] H. Wielandt. Beiträge zur mathematischen Behandlung komplexer Eigenwertprobleme, Teil V: Bestimmung höherer Eigenwerte durch gebrochene Iteration. Bericht B 44/J/37, Aerodynamische Versuchsanstalt Göttingen, 1944.
- [28] J. W. S. Rayleigh. Some General Theorems relating to Vibrations. Proceedings of the London Mathematical Society, Vol. 4, No. 1, pp. 357–368, 1873.
- [29] A. V. Knyazev. Toward the Optimal Preconditioned Eigensolver: Locally Optimal Block Preconditioned Conjugate Gradient Method. SIAM Journal on Scientific Computing, Vol. 23, No. 2, pp. 517–541, 2001.
- [30] E. Suetomi and H. Sekimoto. Conjugate Gradient Like Methods and Their Application to Eigenvalue Problems for Neutron Diffusion Equation. Annals of Nuclear Energy, Vol. 18, No. 4, pp. 205–227, 1991
- [31] H. R. Rutishauser. Computational Aspects of F. L. Bauser's Simultaneous Iteration Method. Numerische Mathematik, Vol. 13, No. 1, pp. 4–13, 1969.
- [32] C. Lanczos. An Iteration Method for the Solution of the Eigenvalue Problem of Linear Differential and Integral Operators. Journal of Research of the National Bureau of Standards, Vol. 45, No. 4, pp. 255–282, 1950.
- [33] W. E. Arnoldi. The Principle of Minimized Iterations in the Solution of the Matrix Eigenvalue Problems. Quarterly of Applied Mathematics, Vol. 9, No. 17, pp. 17–29, 1951.
- [34] O. Axelsson. A Survey of Preconditioned Iterative Methods for Linear Systems of Equations. BIT, Vol. 25, No. 1, pp. 166–187, 1985.
- [35] I. Gustafsson. A Class of First Order Factorization Methods. BIT, Vol. 18, No. 2, pp. 142–156, 1978.

- [36] K. Nakajima, H. Nakamura, and T. Tanahashi. Parallel Iterative Solvers with Localized ILU Preconditioning. Lecture Notes in Computer Science 1225, pp. 342–350, 1997.
- [37] Y. Saad. ILUT: A Dual Threshold Incomplete LU Factorization. Numerical Linear Algebra with Applications, Vol. 1, No. 4, pp. 387–402, 1994.
- [38] Y. Saad, et al. ITSOL: ITERATIVE SOLVERS Package. http://www-users.cs.umn.edu/~saad/software/ITSOL/.
- [39] N. Li, Y. Saad, and E. Chow. Crout Version of ILU for General Sparse Matrices. SIAM Journal on Scientific Computing, Vol. 25, No. 2, pp. 716–728, 2003.
- [40] T. Kohno, H. Kotakemori, and H. Niki. Improving the Modified Gauss-Seidel Method for Z-matrices. Linear Algebra and its Applications, Vol. 267, pp. 113–123, 1997.
- [41] A. Fujii, A. Nishida, and Y. Oyanagi. Evaluation of Parallel Aggregate Creation Orders: Smoothed Aggregation Algebraic Multigrid Method. High Performance Computational Science and Engineering, pp. 99–122, Springer, 2005.
- [42] K. Abe, S. Zhang, H. Hasegawa, and R. Himeno. A SOR-base Variable Preconditioned CGR Method (in Japanese). Transactions of the JSIAM, Vol. 11, No. 4, pp. 157–170, 2001.
- [43] R. Bridson and W. P. Tang. Refining an Approximate Inverse. Journal of Computational and Applied Mathematics, Vol. 123, No. 1-2, pp. 293–306, 2000.
- [44] T. Chan and T. Mathew. Domain Decomposition Algorithms. Acta Numerica, Vol. 3, pp. 61–143, 1994.
- [45] M. Dryja and O. B. Widlund. Domain Decomposition Algorithms with Small Overlap. SIAM Journal on Scientific Computing, Vol. 15, No. 3, pp. 604–620, 1994.
- [46] H. Kotakemori, H. Hasegawa, and A. Nishida. Performance Evaluation of a Parallel Iterative Method Library using OpenMP. Proceedings of the 8th International Conference on High Performance Computing in Asia Pacific Region, pp. 432–436, IEEE, 2005.
- [47] H. Kotakemori, H. Hasegawa, T. Kajiyama, A. Nukada, R. Suda, and A. Nishida. Performance Evaluation of Parallel Sparse Matrix-Vector Products on SGI Altix 3700. Lecture Notes in Computer Science 4315, pp. 153–163, Springer, 2008.
- [48] D. H. Bailey. A Fortran-90 Double-Double Library. http://crd-legacy.lbl.gov/~dhbailey/mpdist/.
- [49] Y. Hida, X. S. Li, and D. H. Bailey. Algorithms for Quad-Double Precision Floating Point Arithmetic. Proceedings of the 15th Symposium on Computer Arithmetic, pp. 155–162, 2001.
- [50] T. Dekker. A Floating-Point Technique for Extending the Available Precision. Numerische Mathematik, Vol. 18, No. 3, pp. 224–242, 1971.
- [51] D. E. Knuth. The Art of Computer Programming: Seminumerical Algorithms, Vol. 2. Addison-Wesley, 1969.
- [52] D. H. Bailey. High-Precision Floating-Point Arithmetic in Scientific Computation. Computing in Science and Engineering, Vol. 7, No. 3, pp. 54–61, IEEE, 2005.
- [53] Intel Fortran Compiler for Linux Systems User's Guide, Vol I. Intel Corporation, 2004.
- [54] H. Kotakemori, A. Fujii, H. Hasegawa, and A. Nishida. Implementation of Fast Quad Precision Operation and Acceleration with SSE2 for Iterative Solver Library (in Japanese). IPSJ Transactions on Advanced Computing Systems, Vol. 1, No. 1, pp. 73–84, 2008.
- [55] R. Courant and D. Hilbert. Methods of Mathematical Physics. Wiley-VCH, 1989.

- [56] C. Lanczos. The Variational Principles of Mechanics, 4th Edition. University of Toronto Press, 1970.
- [57] J. H. Wilkinson. The Algebraic Eigenvalue Problem. Oxford University Press, 1988.
- [58] D. M. Young. Iterative Solution of Large Linear Systems. Academic Press, 1971.
- [59] G. H. Golub and C. F. Van Loan. Matrix Computations, 3rd Edition. The Johns Hopkins University Press, 1996.
- [60] J. J. Dongarra, I. S. Duff, D. C. Sorensen, and H. A. van der Vorst. Solving Linear Systems on Vector and Shared Memory Computers. SIAM, 1991.
- [61] Y. Saad. Numerical Methods for Large Eigenvalue Problems. Halsted Press, 1992.
- [62] R. Barrett, et al. Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods. SIAM, 1994.
- [63] Y. Saad. Iterative Methods for Sparse Linear Systems. Second Edition. SIAM, 2003.
- [64] A. Greenbaum. Iterative Methods for Solving Linear Systems. SIAM, 1997.
- [65] Z. Bai, et al. Templates for the Solution of Algebraic Eigenvalue Problems. SIAM, 2000.
- [66] J. H. Wilkinson and C. Reinsch. Handbook for Automatic Computation, Vol. 2: Linear Algebra. Grundlehren Der Mathematischen Wissenschaften, Vol. 186, Springer, 1971.
- [67] B. T. Smith, J. M. Boyle, Y. Ikebe, V. C. Klema, and C. B. Moler. Matrix Eigensystem Routines: EISPACK Guide, 2nd ed. Lecture Notes in Computer Science 6, Springer, 1970.
- [68] B. S. Garbow, J. M. Boyle, J. J. Dongarra, and C. B. Moler. Matrix Eigensystem Routines: EISPACK Guide Extension. Lecture Notes in Computer Science 51, Springer, 1972.
- [69] J. J. Dongarra, J. R. Bunch, G. B. Moler, and G. M. Stewart. LINPACK Users' Guide. SIAM, 1979.
- [70] J. R. Rice and R. F. Boisvert. Solving Elliptic Problems Using ELLPACK. Springer, 1985.
- [71] E. Anderson, et al. LAPACK Users' Guide. 3rd ed. SIAM, 1987.
- [72] J. Dongarra, A. Lumsdaine, R. Pozo, and K. Remington. A Sparse Matrix Library in C++ for High Performance Architectures. Proceedings of the Second Object Oriented Numerics Conference, pp. 214–218, 1992.
- [73] I. S. Duff, R. G. Grimes, and J. G. Lewis. Users' Guide for the Harwell-Boeing Sparse Matrix Collection (Release I). Technical Report TR/PA/92/86, CERFACS, 1992.
- [74] Y. Saad. SPARSKIT: A Basic Tool Kit for Sparse Matrix Computations, Version 2, 1994. http://www-users.cs.umn.edu/~saad/software/SPARSKIT/.
- [75] A. Geist, et al. PVM: Parallel Virtual Machine. MIT Press, 1994.
- [76] R. Bramley and X. Wang. SPLIB: A Library of Iterative Methods for Sparse Linear System. Technical Report, Department of Computer Science, Indiana University, 1995.
- [77] R. F. Boisvert, et al. The Matrix Market Exchange Formats: Initial Design. Technical Report NISTIR 5935, National Institute of Standards and Technology, 1996.
- [78] L. S. Blackford, et al. ScaLAPACK Users' Guide. SIAM, 1997.
- [79] R. B. Lehoucq, D. C. Sorensen, and C. Yang. ARPACK Users' Guide: Solution of Large-Scale Eigenvalue Problems with Implicitly-Restarted Arnoldi Methods. SIAM, 1998.

- [80] R. S. Tuminaro, et al. Official Aztec User's Guide, Version 2.1. Technical Report SAND99-8801J, Sandia National Laboratories, 1999.
- [81] W. Gropp, E. Lusk, and A. Skjellum. Using MPI, 2nd Edition: Portable Parallel Programming with the Message-Passing Interface. MIT Press, 1999.
- [82] K. Garatani, H. Nakamura, H. Okuda, and G. Yagawa. GeoFEM: High Performance Parallel FEM for Solid Earth. Lecture Notes in Computer Science 1593, pp. 133–140, Springer, 1999.
- [83] S. Balay, et al. PETSc Users Manual. Technical Report ANL-95/11, Argonne National Laboratory, 2004.
- [84] V. Hernandez, J. E. Roman, and V. Vidal. SLEPc: A Scalable and Flexible Toolkit for the Solution of Eigenvalue Problems. ACM Transactions on Mathematical Software, Vol. 31, No. 3, pp. 351–362, 2005.
- [85] M. A. Heroux, et al. An Overview of the Trilinos Project. ACM Transactions on Mathematical Software, Vol. 31, No. 3, pp. 397–423, 2005.
- [86] R. D. Falgout, J. E. Jones, and U. M. Yang. The Design and Implementation of hypre, a Library of Parallel High Performance Preconditioners. Lecture Notes in Computational Science and Engineering 51, pp. 209–236, Springer, 2006.
- [87] B. Chapman, G. Jost, and R. van der Pas. Using OpenMP: Portable Shared Memory Parallel Programming. MIT Press, 2007.
- [88] J. Dongarra and M. Heroux. Toward a New Metric for Ranking High Performance Computing Systems. Technical Report SAND2013-4744, Sandia National Laboratories, 2013.

# A File Formats

This section describes the file formats available for the library. Note that both the upper and lower triangular entries need to be stored irrespective of whether the matrix is symmetric or not in Harwell-Boeing Format.

#### A.1 Extended Matrix Market Format

The Matrix Market format does not support the vector data. The extended Matrix Market format is the extension of the Matrix Market format to handle the matrix and vector data. Assume that the number of nonzero elements of matrix  $A = (a_{ij})$  of size  $M \times N$  is L and that  $a_{ij} = A(I, J)$ . The format is as follows:

```
%%MatrixMarket matrix coordinate real general
                                                   <-- Header
                                                    <-+
%
                                                      | Comment lines with 0 or more lines
%
{\tt M} {\tt N} {\tt L} {\tt B} {\tt X}
                                                    <-- Numbers of rows, columns, and
I1 J1 A(I1,J1)
                                                         nonzero elements (0 or 1) (0 or 1)
I2 J2 A(I2,J2)
                                                      | Row and column number values
                                                      | The index is one-origin
IL JL A(IL, JL)
                                                    <-+
I1 B(I1)
I2 B(I2)
                                                      | Exists only when B=1
                                                      | Row number value
 . . .
IM B(IM)
I1 X(I1)
I2 X(I2)
                                                      | Exists only when X=1
                                                      | Row number value
IM X(IM)
```

The extended Matrix Market format for matrix A and vector b in Equation (A.1) is as follows:

$$A = \begin{pmatrix} 2 & 1 & & \\ 1 & 2 & 1 & & \\ & 1 & 2 & 1 \\ & & 1 & 2 \end{pmatrix} \qquad b = \begin{pmatrix} 0 & & \\ 1 & & \\ 2 & & \\ 3 & & \end{pmatrix}$$
 (A.1)

%%MatrixMarket matrix coordinate real general

```
4 4 10 1 0
1 2 1.00e+00
1 1 2.00e+00
2 3 1.00e+00
2 1
    1.00e+00
2 2
    2.00e+00
3 4 1.00e+00
3 2
    1.00e+00
3 3 2.00e+00
4 4 2.00e+00
4 3 1.00e+00
1 0.00e+00
2 1.00e+00
3 2.00e+00
```

4 3.00e+00

## A.2 Harwell-Boeing Format

The Harwell-Boeing format stores the matrix in the CSC format. Assume that the array value stores the values of the nonzero elements of matrix A, the array index stores the row indices of the nonzero elements and the array ptr stores pointers to the top of each column in the arrays value and index. The format is as follows:

```
Line 1 (A72,A8)
  1 - 72 Title
 73 - 80 Key
Line 2 (5I14)
  1 - 14 Total number of lines excluding header
 15 - 28 Number of lines for ptr
 29 - 42 Number of lines for index
 43 - 56 Number of lines for value
 57 - 70 Number of lines for right-hand side vectors
Line 3 (A3,11X,4I14)
  1 - 3 Matrix type
           Col.1:
             R Real matrix
             C Complex matrix
             P Pattern only (Not supported)
           Col.2:
             S Symmetric (Not supported)
             U Unsymmetric
             H Hermitian (Not supported)
             Z Skew symmetric (Not supported)
             R Rectangular (Not supported)
           Col.3:
             A Assembled
             E Elemental matrices (Not supported)
  4 - 14 Blank space
 15 - 28 Number of rows
 29 - 42 Number of columns
 43 - 56 Number of nonzero elements
 57 - 70 0
Line 4 (2A16,2A20)
  1 - 16 Format for ptr
 17 - 32 Format for index
 33 - 52 Format for value
 53 - 72 Format for right-hand side vectors
Line 5 (A3,11X,2I14) Only presents if there are right-hand side vectors
         right-hand side vector type
           F for full storage
           M for same format as matrix (Not supported)
         G if a starting vector is supplied
         X if an exact solution is supplied
  4 - 14 Blank space
 15 - 28 Number of right-hand side vectors
 29 - 42 Number of nonzero elements
  The Harwell-Boeing format for matrix A and vector b in Equation (A.1) is as follows:
Harwell-Boeing format sample
                                                                     Lis
                                                    4
                                                                  2
            8
                         1
                                       1
RUA
                                                   10
                                                                  4
(11i7)
               (13i6)
                               (3e26.18)
                                                  (3e26.18)
```

```
F
                                      0
     1
            3
               1
                                2
                                      3
  2.00000000000000000E+00
                         1.0000000000000000E+00 1.00000000000000E+00
  2.00000000000000000E+00
                          1.0000000000000000E+00 1.00000000000000E+00
  2.00000000000000000E+00
                          1.0000000000000000E+00
                                                  1.0000000000000000E+00
  2.0000000000000000E+00
  0.0000000000000000E+00
                                                 2.00000000000000000E+00
                          1.0000000000000000E+00
  3.0000000000000000E+00
```

### A.3 Extended Matrix Market Format for Vectors

The extended Matrix Market format for vectors is the extension of the Matrix Market format to handle the vector data. Assume that vector  $b = (b_i)$  is a vector of size N and that  $b_i = B(I)$ . The format is as follows:

```
      %%MatrixMarket vector coordinate real general
      <-- Header</td>

      %
      <-+</td>

      %
      | Comment lines with 0 or more lines

      %
      <-+</td>

      N
      <-- Number of rows</td>

      I1 B(I1)
      <-+</td>

      I2 B(I2)
      | Row number value

      . . .
      | The index is one-origin

      IN B(IN)
      <-+</td>
```

The extended Matrix Market format for vector b in Equation (A.1) is as follows:

```
%%MatrixMarket vector coordinate real general
4
1 0.00e+00
2 1.00e+00
3 2.00e+00
4 3.00e+00
```

### A.4 PLAIN Format for Vectors

The PLAIN format for vectors is designed to write vector values in order. Assume that vector  $b = (b_i)$  is a vector of size N and that  $b_i$  is equal to B(I). The format is as follows:

The PLAIN format for vector b in Equation (A.1) is as follows:

```
0.00e+00
1.00e+00
2.00e+00
3.00e+00
```